A DISSIPATIVE MODEL FOR HYDROGEN STORAGE: EXISTENCE AND REGULARITY RESULTS

ELISABETTA CHIODAROLI

Abstract. We prove global existence of a solution to an initial and boundary value problem for a highly nonlinear PDE system. The problem arises from a thermomechanical dissipative model describing hydrogen storage by use of metal hydrides. In order to treat the model from an analytical point of view, we formulate it as a phase transition phenomenon thanks to the introduction of a suitable phase variable. Continuum mechanics laws lead to an evolutionary problem involving three state variables: the temperature, the phase parameter and the pressure. The problem thus consists of three coupled partial differential equations combined with initial and boundary conditions. Existence and regularity of the solutions are here investigated by means of a time discretization-a priori estimates-passage to the limit procedure joined with compactness and monotonicity arguments.

1. Introduction

The paper deals with a thermo-mechanical model describing hydrogen storage in terms of metal hydrides. Hydrogen storage basically implies a reduction in the enormous volume of hydrogen gas; 1 kg of hydrogen at ambient temperature and atmospheric pressure has a volume of 11 m^3. There are basically six methods in order to store hydrogen reversibly with a high volumetric and gravimetric density: hydrogen gas, liquid hydrogen, physisorption, complex, chemical hydrides, metal hydrides. This latter technique exploits the possibility of many metals to absorb hydrogen: such metals and alloys are able to react spontaneously with hydrogen and they can store a large amount of it. These materials, either a defined compound or a solid solution, are designed as metal hydrides: their use in the hydrogen storage is of interest in terms of safety, global yield and long-time storage. Energetic and industrial applications warrant this interest. Indeed, hydrogen is foreseen to be a clean and efficient energy carrier for the future (cf. [16]). Nowadays, energetic needs are mainly covered by fossil energies leading to pollutant emissions mostly responsible for global warming. Hydrogen stands among the best solutions to the shortage of fossil energies and to the greenhouse effect, in particular for energy transportation.

Our research moves in the direction of providing a predictive theory for the storage of hydrogen by use of metal hydrides (cf. [16]). To this aim our analysis refers to the thermo-mechanical model introduced by E. Bonetti, M. Frémond and C. Lexcellent in [7] and it complements their results. Following the usual approach of Thermodynamics, Bonetti, Frémond and Lexcellent have derived the governing equilibrium equations. The analytical formulation of the problem they obtained was new and, to the best of our knowledge, no other related results can be found in the literature. Our work is attempted to go one step further both in modeling and analytical aspects of hydrogen storage by use of metal hydrides (cf. [9]). The problem we will deal with results from a phase transition model and is formulated via the classical principles of Continuum Mechanics. The related strongly nonlinear PDE system has been investigated, from the point of view of existence and regularity of the solutions.

In order to get acquainted with the phenomenon, we recall some of its basic features. Some metals are able to absorb hydrogen atoms and combine with them to form solid solutions. We assume the existence of two solid solutions: the α-phase and the β-phase. The presence of one phase with respect to the other depends on the pressure of the hydrogen. To provide a good mechanical model to be analytically treated from the point of view of existence and regularity of solutions, it seems useful to exploit the theory of phase transitions. We choose the volume fraction of one of the phases as a state quantity and we denote it by χ. Hence, χ satisfies the relation

$$\chi \in [0,1], \tag{1.1}$$

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and, assuming that no voids appear in the mixture, the volume fraction of the other phase is simply given by $1-\chi$. More precisely, if $\chi = 1$ we have the α-phase, if $\chi = 0$ we have the β-phase, and if $\chi \in (0,1)$ both phases are present in suitable proportions. The state variables of the model are the absolute temperature θ, the hydrogen pressure p, and the phase parameter χ along with its gradient $\nabla\chi$ accounting for local interactions between the different phases. Constitutive relations for the state quantities will be chosen in such a way that the principles of Thermodynamics are satisfied. Finally, to describe the thermo-mechanical evolution of the system, a pseudo-potential of dissipation will be considered. The constitutive equations will be substantially recovered as in [7]. Nevertheless, some improvements will be introduced in the model. Indeed, in [7] the PDE system is written by neglecting dissipative effects and microscopic movements in the power of interior forces. Our approach will be different, as we aim to derive the complete dissipative model accounting for microscopic velocities and diffusive phase transformations. Moreover, [7] is concerned with the study of a weaker formulation of the system: in this framework the authors have been able to prove a global existence result holding for $n = 3$. We complement their results. Indeed, in our framework we can prove a more general existence result in the three-dimensional setting. Moreover, by refining the assumptions on the data, we are able to show further regularities for the solutions to our problem. Some related analytical results can be found for models describing irreversible phase transition phenomena. In particular, we refer to [17] and [19]: these papers deal with nonlinear systems of PDEs governing the evolution of two unknown fields (θ and χ) and prove some existence results. We refer also to [5] and [6], both concerning the analysis of a dissipative Frémond model for shape memory alloys. The problem therein is quite similar to our both for modeling aspects and analytical investigation: many techniques and analytical tools from [5] and [6] have inspired our proofs.

Now, let us introduce the complete thermo-mechanical model describing hydrogen storage by use of metal hydrides and including dissipative effects and miscroscopic velocities in the constitutive equations as well as microscopic forces in the principle of virtual power. Then, we state an initial and boundary value problem for the obtained model.

We write the model in terms of the state variables θ, p and χ. In order to achieve a precise description of the phenomenon, we take into account both the equilibrium and the evolution of the system, which are characterized by two functionals: the free energy Ψ, defined on state variables, and the pseudo-potential of dissipation Φ, defined on dissipative variables. Constitutive relations for the involved thermo-mechanical quantities are chosen in accordance with the principles of Thermodynamics.

We preface our discussion by defining the hydrogen density ρ_H and the total density ρ (in what follows we take $\rho = 1$). Thus, letting c_H be the capacity of the hydrogen, we have that $c_H = \rho_H(\rho - \rho_H)^{-1}$, i.e.,

$$\rho_H = \rho \frac{c_H}{1 + c_H} = \frac{1}{\tau},$$

where τ stands for the hydrogen's specific volume.

Now, we introduce the free energy function $\Psi(\theta, \tau, \chi, \nabla\chi)$. By thermodynamical and duality arguments it follows that the free energy is concave with respect to θ, while we assume that it is convex with respect to τ, χ, and $\nabla\chi$. Thus, as Ψ is convex with respect to τ, we can introduce the dual function Ψ^* of Ψ as follows:

$$\Psi^*(\theta, \zeta, \chi, \nabla\chi) = \sup_s \{\zeta s - \Psi(\theta, s, \chi, \nabla\chi)\}.$$

Next, we define the pressure p connected with the hydrogen's specific volume τ by the following relation

$$-p := \frac{\partial\Psi}{\partial\tau}(\theta, \tau, \chi, \nabla\chi). \tag{1.2}$$

This corresponds to setting

$$\tau = \frac{\partial\Psi^*}{\partial(-p)}(\theta, -p, \chi, \nabla\chi) = -\frac{\partial\Psi^*}{\partial p}(\theta, -p, \chi, \nabla\chi).$$

Thus, if we assume sufficient regularity for the functionals we get

$$\Psi^*(\theta, -p, \chi, \nabla\chi) = -p\tau - \Psi(\theta, \tau, \chi, \nabla\chi).$$

Finally, we deal with the *enthalpy functional* $G(\theta, p, \chi, \nabla\chi)$ defined in terms of the Legendre-Fenchel transformation of Ψ with respect to the specific volume τ. More precisely, the enthalpy $G(p)$ is defined by

$$G(p) := -\Psi^*(-p)$$

so that it results

$$G(\theta, p, \chi, \nabla\chi) = \Psi(\theta, \tau, \chi, \nabla\chi) + p\tau. \tag{1.3}$$

In particular, we recover that G is concave with respect to p and θ, while it is convex with respect to χ and $\nabla\chi$.

Then, we make precise the constitutive relations holding for the entropy s, the specific volume τ, and the internal energy e (see (1.3)). We have

$$s = -\frac{\partial\Psi}{\partial\theta} = -\frac{\partial G}{\partial\theta}, \tag{1.4}$$

$$\tau = \frac{\partial G}{\partial p}, \tag{1.5}$$

$$e = \Psi + \theta s = G - p\tau + \theta s. \tag{1.6}$$

The fundamental balance laws of Continuum Mechanics, written in a smooth bounded domain $\Omega \subset \mathbb{R}^n$ during a finite time interval $[0, T]$ are: the momentum balance, the energy balance and the mass balance. In the following we will denote the time derivative of any function f by the symbol f_t. At first, by the principle of virtual power written for microscopic movements (i.e., neglecting any virtual macroscopic velocity), we recover an equilibrium equation for the interior forces, which formally correspond to the balance of the momentum seen as a microscopic equilibrium equation. Namely, in absence of external actions, we readily get

$$B - \operatorname{div} \boldsymbol{H} = 0 \quad \text{in } \Omega, \tag{1.7}$$

coupled with the boundary condition

$$\boldsymbol{H} \cdot \boldsymbol{n} = 0 \quad \text{on } \Gamma, \tag{1.8}$$

where $\Gamma = \partial\Omega$. From (1.7)-(1.8) we can deduce the mechanical meaning of the vector $\boldsymbol{H}$, which indicates a work flux vector, while B is a scalar quantity collecting microscopic forces. In case when macroscopic deformations are described by $-\tau_t$, we address the following energy balance equation

$$e_t + \operatorname{div} \boldsymbol{q} = r + B\chi_t + \boldsymbol{H} \cdot \nabla\chi_t - p\tau_t \quad \text{in } \Omega, \tag{1.9}$$

where by e we denote the internal energy as defined in (1.6); $\boldsymbol{q}$ represents the heat flux vector, for which we will state later a suitable boundary condition. The right hand side of (1.9) accounts for heat sources induced by mechanical and external actions. More precisely, r is an exterior heat source, while heat sources induced by microscopic forces are collected by the terms involving the quantities B and $\boldsymbol{H}$. The presence of microscopic mechanically induced heat sources in (1.9) is justified by a generalization of the principle of virtual power in which interior microscopic forces and motions are also considered, as they are responsible for the phase transition (cf. [12]). Finally (1.9) is complemented with a Neumann boundary condition

$$-\boldsymbol{q} \cdot \boldsymbol{n} = 0 \quad \text{on } \Gamma, \tag{1.10}$$

where $\boldsymbol{n}$ stands for the normal unit vector on the boundary $\Gamma = \partial\Omega$. This corresponds to prescribe a null heat flux through the boundary Γ. Here, and in the remainder of the work, we assume small perturbations. Hence, letting the mass of the hydrogen that is not in the solid solutions keep constant, the hydrogen mass balance reads as follows

$$(\rho_H)_t + \operatorname{div} \boldsymbol{v} = 0 \quad \text{in } \Omega, \tag{1.11}$$

where $\boldsymbol{v}$ is the hydrogen mass flux. Then we combine (1.11) with the following boundary condition

$$-\boldsymbol{v} \cdot \boldsymbol{n} + \gamma p = 0 \quad \text{on } \Gamma, \quad \gamma > 0, \tag{1.12}$$

by which we require that the hydrogen flux through the boundary is proportional to the difference between the exterior and the interior pressure (here the exterior pressure is chosen equal to 0).

In order to describe the thermo-mechanical evolution of the system and to include dissipation in the model by following the approach by Moreau (cf. [20]), we introduce a pseudo-potential of dissipation Φ depending on χ_t, $\nabla\chi_t$ and $\nabla\theta$. We recall the properties of Φ:

$$\Phi \geq 0, \qquad \Phi(\mathbf{0}) = 0, \qquad \Phi \quad \text{is convex.} \tag{1.13}$$

By (1.13), it turns out that the subdifferential $\partial\Phi$ is a maximal monotone operator with $\mathbf{0} \in \partial\Phi(\mathbf{0})$. In particular, it follows that

$$\partial\Phi(\chi_t, \nabla\chi_t, \nabla\theta) \cdot (\chi_t, \nabla\chi_t, , \nabla\theta) \geq 0. \tag{1.14}$$

Now, we are in the position to exhibit the constitutive relations for B and $\boldsymbol{H}$, in terms of G and Φ. Unlike Bonetti, Frémond and Lexcellent (see [7]) we include dissipative effects both in B and in $\boldsymbol{H}$ and we prescribe them to be given by the sum of a dissipative and a non-dissipative contribution. Let us introduce a useful notation: nd in the apex is used for pointing out nondissipative contributions, while d stands for dissipative ones. Namely, we specify B as

$$B = B^{\mathrm{nd}} + B^{\mathrm{d}} = \frac{\partial G}{\partial \chi} + \frac{\partial \Phi}{\partial \chi_t}, \tag{1.15}$$

and $\boldsymbol{H}$ as

$$\boldsymbol{H} = \boldsymbol{H}^{\mathrm{nd}} + \boldsymbol{H}^{\mathrm{d}} = \frac{\partial G}{\partial(\nabla\chi)} + \frac{\partial \Phi}{\partial(\nabla\chi_t)}. \tag{1.16}$$

The heat flux vector $\boldsymbol{q}$ is assumed to fulfil the standard Fourier law

$$\boldsymbol{q} = -k_0 \nabla\theta, \tag{1.17}$$

where $k_0 > 0$. Let us anticipate that, by a suitable choice of Φ, the heat flux can be expressed by use of the pseudo-potential of dissipation. Finally, we set the following relation for the hydrogen mass flux

$$\boldsymbol{v} = -\lambda \nabla p, \tag{1.18}$$

for $\lambda > 0$ (take, e.g., $\lambda = 1$).

Let us come to the functionals that describe the equilibrium and the evolution of the system. As first we set the enthalpy functional G as

$$G(\theta, p, \chi, \tau) = a \log p + b\chi(\log p - \log p_e) - c_p \theta \log\theta + \frac{\delta}{2}|\nabla\chi|^2 + I_{[0,1]}(\chi), \tag{1.19}$$

where $c_p > 0$, $\delta > 0$ and $I_{[0,1]}(\chi) := 0$ if $\chi \in [0,1]$ and $I_{[0,1]}(\chi) := +\infty$ otherwise. By p_e in (1.19) we denote the *equilibrium* or *Plateau pressure* which is strongly temperature dependent. In accordance with physical experience, we let $a > 0$ and $b > 0$ (take, e.g., $a = b = 1$). Hence, experiments show that for θ sufficiently large the Van't Hoff law holds (see [16]), i.e.,

$$\log p_e = -c_1 \frac{1}{\theta} + c_2, \tag{1.20}$$

where c_1 and c_2 are positive constants. However, as we have already pointed out, the enthalpy G has to be concave with respect to the temperature, on the whole temperature interval. Thus we complement relation (1.20) by setting

$$\log p_e = h(\theta), \tag{1.21}$$

where h is a sufficiently smooth function, e.g.

$$\begin{aligned} &h(\theta) = -c_1\theta^{-1} + c_2 \quad \text{for } \theta \text{ sufficiently large, say } \theta \geq \theta_*, \\ &h(\theta) = \tilde{h}(\theta) \quad \text{for } \theta_{**} \leq \theta < \theta_*, \\ &h(\theta) = \text{constant} \quad \text{for } \theta < \theta_{**}, \end{aligned} \tag{1.22}$$

with $\tilde{h}(\theta)$ suitably defined to yield $h \in C^2(\mathbb{R})$. Moreover, $\tilde{h}(\theta)$ and other values have to be chosen in such a way that

$$\frac{\partial^2 G}{\partial\theta^2} = -b\chi h''(\theta) - \frac{c_p}{\theta} < 0. \tag{1.23}$$

Indeed, (1.23) ensures that G is concave with respect to temperature, which is necessary to get the thermodynamic consistency of the model. As it will be clear in what follows, (1.23) is in direct relationship with some assumptions on h concerning the analytical solvability of the resulting heat equation.

In order to derive the model in a thermodynamic frame we have to fulfil the second law of Thermodynamics in the form of the Clausius-Duhem inequality. To this aim, it is convenient to introduce the heat flux vector $\boldsymbol{q}$ formally as a dissipative quantity defined by the pseudopotential of dissipation Φ. Thus, we set

$$\Phi = \frac{\mu}{2}|\chi_t|^2 + \frac{\nu}{2}|\nabla\chi_t|^2 + \frac{k_0}{2\theta}|\nabla\theta|^2, \tag{1.24}$$

for $k_0 > 0$. Hence, we define a new dissipative quantity

$$\boldsymbol{Q}^d = -\frac{\partial \Phi}{\partial(\nabla\theta)} = -\frac{k_0}{\theta}\nabla\theta, \tag{1.25}$$

so that letting

$$\boldsymbol{q} = \theta \boldsymbol{Q}^d \tag{1.26}$$

yields the Fourier relation (1.17). Now, we point out that by use of the chain rule in (1.9) and the above constitutive relations (1.4)-(1.6), (1.15)-(1.18), (1.25)-(1.26), we can equivalently rewrite the energy balance (1.9) as

$$\theta\left(s_t + \operatorname{div}\boldsymbol{Q}^{\mathrm{d}} - \frac{r}{\theta}\right) = -\boldsymbol{Q}^{\mathrm{d}}\cdot\nabla\theta + B^{\mathrm{d}}\cdot\chi_t + \boldsymbol{H}^{\mathrm{d}}\cdot\nabla\chi_t. \tag{1.27}$$

Thus, after observing that by (1.15), (1.16) and (1.25) the right hand side of (1.27) corresponds to

$$\left(\frac{\partial\Phi}{\partial\chi_t}, \frac{\partial\Phi}{\partial\nabla\chi_t}, \frac{\partial\Phi}{\partial\nabla\theta}\right)\cdot(\chi_t, \nabla\chi_t, \nabla\theta), \tag{1.28}$$

we get, thanks to (1.14),

$$-\boldsymbol{Q}^{\mathrm{d}}\cdot\nabla\theta + B^{\mathrm{d}}\cdot\chi_t + \boldsymbol{H}^{\mathrm{d}}\cdot\nabla\chi_t \geq 0. \tag{1.29}$$

Finally, dividing (1.27) by the absolute temperature θ yields the Clausius-Duhem inequality ensuring thermodynamic consistency, namely

$$s_t + \operatorname{div}\boldsymbol{Q}^{\mathrm{d}} - \frac{r}{\theta} \geq 0. \tag{1.30}$$

Remark 1.1. *Indeed, we have to remark that all the addends in* (1.29) *turn out to be non-negative. In particular, we have*

$$-\boldsymbol{Q}^d\cdot\nabla\theta \geq 0 \tag{1.31}$$

$$B^d\cdot\chi_t \geq 0, \tag{1.32}$$

$$\boldsymbol{H}^d\cdot\nabla\chi_t \geq 0. \tag{1.33}$$

Thanks to (1.31)-(1.32)*, if we take $\nu = 0$ in* (1.24)*, the model still fulfils the Clausius-Duhem inequality. Indeed, letting $\nu = 0$ in* (1.24) *corresponds to neglecting dissipative effects in $\boldsymbol{H}$ (see* (1.16)*): this choice would lead to the model derived by Bonetti, Frémond and Lexcellent in* [7] *which actually is thermodynamically consistent.*

Now, we can write the system of PDE's in terms of the unknowns, by substituting in (1.7), (1.9) and (1.11), the constitutive equations of the model specified by enthalpy and pseudo-potential of dissipation. In particular, we write the vectors of microscopic forces (1.15) and (1.16) on account of (1.19) and (1.24)

$$B = b(\log p - h(\theta)) + \partial I_{[0,1]}(\chi) + \mu\chi_t, \tag{1.34}$$

$$\boldsymbol{H} = \delta\nabla\chi + \nu\nabla\chi_t. \tag{1.35}$$

Let us note that $\partial I_{[0,1]}$ in (1.34) stands for the subdifferential of the indicator function of the convex $[0,1] \subset \mathbb{R}$ and it is obtained as a generalized derivative with respect to χ of the non smooth function $I_{[0,1]}$ in (1.19). Actually, in our analysis we will consider a more general maximal monotone graph β in place of $\partial I_{[0,1]}$, still with non negative and bounded domain. Thus, the complete PDE system originating from (1.9), (1.11) and (1.7) is written in $Q := \Omega \times (0,T)$ as follows:

$$(bh''(\theta)\theta\chi + c_p)\theta_t - k_0\Delta\theta = r + \mu\chi_t^2 + \nu\left|\nabla\chi_t\right|^2 - b\theta h'(\theta)\chi_t, \tag{1.36}$$

$$\mu\chi_t - \nu\Delta\chi_t - \delta\Delta\chi + \xi = -b(-h(\theta) + \log p), \tag{1.37}$$

$$\xi \in \beta(\chi), \tag{1.38}$$

$$\left(\frac{p}{a + b\chi}\right)_t - \lambda\Delta p = 0. \tag{1.39}$$

Then (1.36)-(1.39) are combined with initial conditions

$$\theta(0) = \theta_0, \tag{1.40}$$

$$\chi(0) = \chi_0, \tag{1.41}$$

$$p(0) = p_0, \tag{1.42}$$

and the natural boundary conditions (∂_n is the normal derivative operator on the boundary Γ)

$$k_0\partial_n\theta = 0, \tag{1.43}$$

$$\nu\,(\partial_n\chi)_t + \delta\partial_n\chi = 0, \tag{1.44}$$

$$\lambda\partial_n p + \gamma p = 0, \tag{1.45}$$

on $\Gamma \times (0,T)$. Observe that the unusual boundary condition (1.44) results from the position (1.35) and, however, it is perfectly equivalent to the standard boundary condition $\partial_n\chi = 0$ whenever the compatibility condition $\partial_n\chi_0 = 0$ holds true on Γ, as in our approach (cf. (2.34)).

Let us point out to the reader that we deal with a slightly modified version of the system (1.36)-(1.39), as in equation (1.36) we consider $\nu = 0$ and neglect exterior heat sources ($r = 0$). From a mechanical perspective, letting $\nu = 0$ in (1.36) corresponds to require that dissipative effects on the gradients of the phases are negligible in the power of interior forces with respect to the other mechanically induced heat sources, which is reasonable in the framework of the small perturbations assumption. Thus in the sequel, by abuse of notation, we will refer to (1.36) but considering $\nu = 0$ and $r = 0$. Moreover, as our existence theorem for weak solutions to problem (1.36)-(1.45) does not ensure the pointwise validity of (1.37), we have to consider an extension of inclusion (1.38) in the framework of a pair of spaces in duality.

The above formulation of the problem of hydrogen storage complements the model advanced in [7]. In particular, the quadratic term χ_t^2 in (1.36) is new, as well as $\Delta\chi_t$ in (1.37). Let us note that the solvability of the resulting PDE system, written as a phase-field problem, turns out to be interesting from the analytical point of view. Indeed, the system (1.36)-(1.45) is highly nonlinear and solving it (in some suitable sense) requires non trivial analytical tools. This is mainly due to the coupling of higher-order nonlinear contributions involving the unknowns, a maximal monotone graph and a quadratic dissipative term for the phase parameter, a logarithmic term involving the pressure. More precisely, in the parabolic equation (1.36) the specific heat is a nonlinear function: to ensure coerciveness, we need to prescribe a suitable assumption on the function h. Dealing with the equation governing the evolution of the pressure, we have to combine the regularity of the function χ and the pressure p, mainly to control the nonlinear evolution term. Finally, it is worth observing that the pressure has a major role in the evolution of the phase through the presence of its logarithm as a source in the corresponding evolution inclusion (see (1.37)). The logarithm is easily controlled for high values of the pressure, whenever we are able to control p, but it degenerates as $p \searrow 0$. Thus, our proof present some ad hoc estimates for (1.39) to handle this nonlinearity in the phase equation.

Here is the outline of the paper. In the next section, we introduce an equivalent abstract formulation of the n-problem (1.36)-(1.39), on account of the initial and boundary conditions (1.40)-(1.45). In particular, we will focus our investigation on the three-dimensional problem as it is more meaningful from the physical point of view. At first, under suitable assumptions on the function h in (1.21), we can state a global existence result (Theorem 2.3) holding for $\nu = 0$ in (1.36). Finally, under refined assumptions, we establish some further regularities for the state variables and the positivity of the temperature (Theorems 2.4, 2.5 and 2.6).

The existence result is proved in Sections 3 − 4 − 5 by exploiting a semi-implicit time discretization scheme combined with an a priori estimate-passage to the limit procedure. In section 4, we prove the positivity of the temperature and further regularities for the state variables, by performing suitable a priori estimates on the solutions of the problem. In the Appendix, we present some results we will refer to in our investigation.

2. The abstract problem: main results

Our analysis refers to an abstract version of the problem (1.36)-(1.45). We render the physical constants to 1 (i.e., $a = b = c_p = \lambda = k_0 = \delta = \mu = \gamma = 1$). Next, we start by listing the main mathematical hypotheses of our work. At first, we want to specify β: we introduce a convex, lower semicontinuous and proper function

$$\hat\beta : \mathbb{R} \to (-\infty, +\infty] \tag{2.1}$$

satisfying the following property

$$\operatorname{int} D(\hat\beta) = (0, \lambda_\beta), \tag{2.2}$$

for some constant $\lambda_\beta > 0$. By $D(\hat\beta)$ we denote the *effective domain* of $\hat\beta$. In addition, we assume that there exists $\chi_* \in (0, \lambda_\beta)$ such that

$$0 = \hat\beta(\chi_*) \le \hat\beta(s) \quad \forall s \in D(\hat\beta). \tag{2.3}$$

Now, we can introduce the subdifferential of $\hat\beta$, i.e.,

$$\beta = \partial\hat\beta; \tag{2.4}$$

then, β turns out to be a *maximal monotone graph* in $\mathbb{R} \times \mathbb{R}$ (we refer to [3] and [8] for basic definitions and properties of maximal monotone operators). Let us note that (2.3) implies $0 \in \beta(\chi_*)$. In the above positions $D = D(\beta)$ denotes the domain of the graph β, i.e., $D = \{r \in \mathbb{R} : \beta(r) \neq \emptyset\}$; we recall that $D \subseteqq D(\hat\beta)$.

Remark 2.1. *The graph β is introduced in order to generalize the graph $\partial I_{[0,1]}$ in the physical model we derived; in particular let us stress that the choice $\beta = \partial I_{[0,1]}$ would force χ to attain values only in $[0,1]$ (see (1.1)). Nonetheless, more general classes of constraints could be admissible for the phase variable than that provided by $\xi \in \partial I_{[0,1]}(\chi)$. In particular, from a mathematical point of view, in this analysis we are able and aim to deal with an arbitrary maximal monotone graph β with domain included in some bounded interval $[0, \lambda_\beta]$.*

According to Remark 2.1, in (1.38) we have considered $\beta(\chi)$ in place of $\partial I_{[0,1]}(\chi)$. Thus, the system (1.36)-(1.39) can be rewritten in Q as follows (recall that $\nu = 0$ and $r = 0$ in (1.36)),

$$(h''(\theta)\theta\chi + 1)\theta_t - \Delta\theta = \chi_t^2 - \theta h'(\theta)\chi_t, \tag{2.5}$$

$$\chi_t - \nu\Delta\chi_t - \Delta\chi + \xi = h(\theta) - \log p, \tag{2.6}$$

$$\xi \in \beta(\chi), \tag{2.7}$$

$$\left(\frac{p}{1+\chi}\right)_t - \Delta p = 0. \tag{2.8}$$

For the sake of clarity, before proceeding, we introduce some useful notation. We set

$$H := L^2(\Omega), \quad V := H^1(\Omega),$$

and identify H with its dual space H', so that

$$V \hookrightarrow H \hookrightarrow V' \tag{2.9}$$

with dense and compact injections. Let $(\cdot,\cdot)$ and $\|\cdot\|$ be the inner product and the corresponding norm in H, and denote by $\langle\cdot,\cdot\rangle$ the duality pairing between V' and V. Hence, we introduce the following abstract operators:

$$\mathcal{A} : V \to V', \qquad \langle \mathcal{A}v, u\rangle = \int_\Omega \nabla v \cdot \nabla u, \qquad u, v \in V \tag{2.10}$$

$$\mathcal{B} : V \to V', \qquad \langle \mathcal{B}v, u\rangle = \int_\Omega \nabla v \cdot \nabla u + \int_\Gamma vu, \qquad u, v \in V. \tag{2.11}$$

Then, to simplify notation, we set

$$W := \{f \in H^2(\Omega) : \partial_n f = 0 \quad \text{on} \quad \Gamma\}.$$

Clearly, we have that $W \subset V$ with compact embedding. Whereas the results we present refer also to lower dimensional space domains we have restricted our investigation to the three-dimensional framework as it is more meaningful from the physical point of view. Thus, let

$$\Omega \subset \mathbb{R}^3 \quad \text{and} \quad Q := \Omega \times (0, T), \tag{2.12}$$

where T is a fixed final time. We assume Ω to be a smooth bounded domain. We associate the functional J_H and J on H and V to the function $\hat\beta$, as follows

$$J_H(v) = \int_\Omega \hat\beta(v) \quad \text{if } v \in H \text{ and } \hat\beta(v) \in L^1(\Omega), \tag{2.13}$$

$$J_H(v) = +\infty \quad \text{if } v \in H \text{ and } \hat\beta(v) \notin L^1(\Omega), \tag{2.14}$$

$$J(v) = J_H(v) \quad \text{if } v \in V. \tag{2.15}$$

As it is well known, J_H and J are convex and lower semicontinuous on H and V respectively. Note that they are also proper since V contains all the constant functions. We denote by $\partial_H J_H : H \to 2^H$ and by $\partial_{V,V'} J : V \to 2^{V'}$ the corresponding subdifferentials. We remind that

$$\begin{aligned} \xi \in & \partial_H J_H(\chi) \quad \text{if and only if} \quad \xi \in H, \\ & \chi \in D(J_H), \quad \text{and} \quad J_H(\chi) \le (\xi, \chi - v) + J_H(v) \quad \forall v \in H \end{aligned} \tag{2.16}$$

$$\begin{aligned} \xi \in & \partial_{V,V'} J(\chi) \quad \text{if and only if} \quad \xi \in V', \\ & \chi \in D(J), \quad \text{and} \quad J(\chi) \le \langle \xi, \chi - v \rangle + J(v) \quad \forall v \in V \end{aligned} \tag{2.17}$$

where $D(\cdot)$ denotes, as above, the *effective domain* for functionals and multivalued operators. Note that $\partial_H J_H : H \to 2^H$ and $\partial_{V,V'} J : V \to 2^{V'}$ are maximal monotone operators. Moreover, observe that for $\chi, \xi \in H$ we have (see, e.g., [8, Ex. 2.1.3, p. 21])

$$\xi \in \partial_H J_H(\chi) \quad \text{if and only if} \quad \xi \in \beta(\chi) \quad \text{almost everywhere in } \Omega. \tag{2.18}$$

On the other hand, one can easily check that the inclusion

$$\partial_H J_H(\chi) \subseteq H \cap \partial_{V,V'} J(\chi) \quad \forall \chi \in V \tag{2.19}$$

holds, just as a consequence of (2.15) (compare (2.17) with (2.16)). Therefore, for $\chi \in V$ and $\xi \in H$, the condition

$$\xi \in \beta(\chi) \quad \text{almost everywhere in } \Omega \tag{2.20}$$

implies

$$\xi \in \partial_{V,V'} J(\chi). \tag{2.21}$$

In addition, if we assume $\chi \in V$, $\xi \in H$ and (2.21), then (2.20) holds (cf. [4]). In particular, on account of (2.19), we achieve the validity of the following equality

$$\partial_H J_H(\chi) = H \cap \partial_{V,V'} J(\chi) \quad \forall \chi \in V. \tag{2.22}$$

Nonetheless, we should observe that (2.22) is false for more general functionals, as one can verify by referring to the example presented in [4].

Now, we are in the position to rewrite the PDE system (2.5)-(2.8), combined with initial and boundary conditions (1.40)-(1.45), in the abstract setting of the triplet (V, H, V'). We have to remark that we are not able here to deal with a strong version of (2.5)-(2.8). In particular we cannot deal with the natural extension of β, i.e. the subdifferential $\partial_H J_H$. Hence, the variational inclusion governing the dynamics of the phase is written in the abstract setting of the $V' - V$ duality pairing. Nonetheless, even if it cannot be stated a.e. in Q, it retains its physical consistence since it forces the phase to attain only meaningful values. Indeed, if $\xi(t) \in \partial_{V,V'} J(\chi(t))$ for almost any $t \in (0,T)$, we have in particular that

$$\chi(t) \in D(\hat{\beta}) \quad \text{a.e. in } \Omega. \tag{2.23}$$

For instance, if we take $\hat{\beta} = I_{[0,1]}$, the abstract relation $\xi(t) \in \partial_{V,V'} J(\chi(t))$ for a.a. $t \in (0,T)$ implies that $\chi(t) \in [0,1]_V$[1], and consequently $\chi \in [0,1]$ a.e. in Q. Thus the system is rewritten, in V' and a.e. in $(0,T)$, as follows:

$$e_t + \mathcal{A}\theta = -h(\theta)\chi_t + \chi_t^2, \tag{2.24}$$

$$e = \theta - \chi(h(\theta) - \theta h'(\theta)), \tag{2.25}$$

$$\chi_t + \mathcal{A}(\nu \chi_t + \chi) + \xi = h(\theta) - \log p, \tag{2.26}$$

$$\xi \in \partial_{V,V'} J(\chi), \tag{2.27}$$

$$u_t + \mathcal{B} p = 0, \tag{2.28}$$

$$u = \frac{p}{1+\chi}. \tag{2.29}$$

Let us note that, by (2.25) and (2.29), we have introduced two new auxiliary variables: e and u. The variable e can be expressed as a function ψ of the variables θ and χ:

$$e = \psi(\theta, \chi) := \theta - \chi(h(\theta) - \theta h'(\theta)). \tag{2.30}$$

[1] By $[0,1]_V$ we denote the convex: $[0,1]_V := \{v \in V : v \in [0,1] \text{ a.e. in } \Omega\}$.

On the other hand, the variable u has a precise physical meaning: it can be interpreted as the normalized hydrogen density. Thanks to (1.40)-(1.42) we are allowed to set the following initial conditions for e and u

$$e(0) = e_0 := \theta_0 - \chi_0(h(\theta_0) - \theta_0 h'(\theta_0)), \tag{2.31}$$

$$u(0) = u_0 := \frac{p_0}{1+\chi_0}. \tag{2.32}$$

Remark 2.2. *We point out that, whenever $\xi \in \partial_{V,V'} J(\chi)$ and $\xi \in H$ a.e. in $(0,T)$ we have that actually $\xi \in \partial_H J_H(\chi)$ a.e. in (0,T), from which one can deduce that $\xi \in \beta(\chi)$ a.e. in Q.*

Now, we set the hypothesis on the data prescribed in the first part of our analysis. Concerning the Cauchy data in (1.40)-(1.42), we assume that

$$\theta_0 \in V, \tag{2.33}$$

$$\chi_0 \in W \cap D(J_H) \tag{2.34}$$

$$p_0 \in V, \quad \log p_0 \in L^1(\Omega). \tag{2.35}$$

Note that (2.35) yields $p_0 > 0$ a.e. in Ω. Moreover, (2.34) implies that $\chi_0 \in D(\hat{\beta})$ a.e. in Ω and in particular:

$$0 \le \chi_0 \le \lambda_\beta \quad \text{a.e. in } \Omega, \tag{2.36}$$

where the value λ_β is introduced in (2.2). Finally, from (2.34)-(2.36) we can deduce that

$$u_0 \in V. \tag{2.37}$$

In fact, the following estimate holds

$$\|u_0\|_V^2 \le C\left(\|p_0\|_V^2 + \|p_0\|_V^2\,\|\nabla\chi_0\|_V^2\right) \le C, \tag{2.38}$$

where we have exploited the continuous embedding $V \subset L^4(\Omega)$.

Hence, we ask for a suitable regularity of the thermal expansion coefficient $h(\theta)$, in agreement with the assumptions leading to the physical consistence of the model (see (1.23)). We require

$$h \in W^{2,\infty}(\mathbb{R}) \cap C^2(\mathbb{R}), \tag{2.39}$$

$$\|h\|_{W^{2,\infty}(\mathbb{R})} + |h'(\zeta)\zeta| \le c_h, \quad |h''(\zeta)\zeta| \le c_h', \quad \forall \zeta \in \mathbb{R}, \tag{2.40}$$

for some positive constants c_h, c_h'. In addition, let $c_s > 0$ such that (recall (2.23) and (2.40))

$$1 + \eta h''(\zeta)\zeta \ge c_s > 0, \quad \forall \eta \in D(\hat{\beta}), \quad \forall \zeta \in \mathbb{R}. \tag{2.41}$$

This correspond to assume that the product $c_h'\lambda_\beta$ is small with respect to 1. The hypotheses we made on h allow us to infer that ψ (see (2.30)) is a bi-lipschitz function of the variable θ. Indeed the following bounds hold (see (2.40)-(2.41))

$$0 < c_s \le \partial_1\psi \le 1 + c_e, \tag{2.42}$$

$$|\partial_2\psi| \le c_h, \tag{2.43}$$

for a positive constant c_e depending on c_h', where $\partial_1\psi$, $\partial_2\psi$ denote the partial derivatives of ψ with respect to first and second variable, respectively. Let us recall that for the initial datum e_0 we have: $e_0 = \psi(\theta_0, \chi_0)$ (see (2.31)). This and the regularity of θ_0 and χ_0 in (2.33)-(2.34), along with the above properties of ψ, easily yield

$$e_0 \in V. \tag{2.44}$$

By use of a semi-implicit time discretization scheme combined with the a priori estimate-passage to the limit procedure, we can prove the following related global existence result.

Theorem 2.3 (**Existence**). *Let* (2.33)-(2.35), (2.37), (2.44) *and* (2.39)-(2.41) *hold. Then there exists a quintuple of functions* (θ, e, χ, p, u) *fulfilling*

$$\theta \in L^\infty(0,T,H) \cap L^2(0,T,V), \tag{2.45}$$

$$e \in W^{1,1}(0,T,V') \cap L^\infty(0,T,H) \cap L^2(0,T,V), \tag{2.46}$$

$$\chi \in H^1(0,T,V) \cap L^\infty(0,T,W) \cap L^\infty(Q), \tag{2.47}$$

$$\hat{\beta}(\chi) \in L^\infty(0,T,L^1(\Omega)), \tag{2.48}$$

$$p \in H^1(0,T,H) \cap L^\infty(0,T,V) \cap L^2(0,T,H^2(\Omega)), \tag{2.49}$$

$$\log p \in L^\infty(0,T,L^1(\Omega)) \cap L^2(0,T,V), \tag{2.50}$$

$$u \in H^1(0,T,H) \cap L^\infty(0,T,V), \tag{2.51}$$

and solving (2.24)-(2.29) *in* V'*, a.e. in* $(0,T)$ *along with* (1.41) *and* (2.31)-(2.32).

The regularities obtained in Theorem 2.3 allow the equation (2.28) to make sense a.e. in $\Omega \times (0,T)$: the same does not hold for (2.24) and (2.26) since the regularities *in space* are not strong enough. But, still dealing with the complete problem (2.24)-(2.29), we can establish some further regularity results for the state variables and, in addition, the positivity of the temperature θ. As first, we can prove some properties for the inverse of the pressure p. To this aim, we need to make an additional assumption on the inverse of the initial datum p_0. Namely, we need $1/p_0 = p_0^{-1} \in H$. Then, the following result holds.

Theorem 2.4 (**Regularity of the pressure**). *Under the same assumptions as in Theorem 2.3, if*

$$\frac{1}{p_0} = p_0^{-1} \in H, \tag{2.52}$$

then the following property holds

$$p^{-1} \in L^\infty(0,T,H) \cap L^2(0,T,V). \tag{2.53}$$

The next result is concerned with improved regularities for the time derivatives of the state variables θ and χ.

Theorem 2.5 (**Further Regularities**). *Let* (2.33)-(2.35), (2.37), (2.44), (2.52) *and* (2.39)-(2.41) *hold. Let the quintuple* (θ, e, χ, p, u) *fulfill* (2.45)-(2.51), (2.53) *and solve* (2.24)-(2.29) *along with* (1.41) *and* (2.31)-(2.32). *If*

$$\chi_0 \in D(\partial_{V,V'} J), \tag{2.54}$$

then it holds that

$$\theta \in H^1(0,T,H) \cap L^\infty(0,T,V), \tag{2.55}$$

$$\chi \in W^{1,\infty}(0,T,V). \tag{2.56}$$

Note that the improved regularity (2.55) for the temperature θ allow us to infer from (2.25) that also the time derivative of the internal variable e belongs to $L^2(0,T,H)$. Therefore, the solutions obtained in Theorem 2.5 fulfil equation (2.24) a.e. in $\Omega \times (0,T)$. Finally, we can establish the positivity of the temperature θ, holding under suitable assumptions on the logarithm of the initial datum θ_0. Indeed, the following theorem holds.

Theorem 2.6 (**Positivity of the temperature**). *Under the same assumptions as in Theorem 2.5, if*

$$\log \theta_0 \in L^1(\Omega), \tag{2.57}$$

then the following properties

$$\log \theta \in L^\infty(0,T,L^1(\Omega)) \cap L^2(0,T,V) \tag{2.58}$$

$$\frac{\chi_t}{\sqrt{\theta}} \in L^2(0,T,H) \tag{2.59}$$

hold.

Clearly, (2.58) ensures the temperature θ to be positive a.e. in Q. Theorems 2.4, 2.5 and 2.6 will be proved by performing some suitable a priori estimates on the solutions of the problem whose existence is stated by Theorem 2.3.

3. Time discretization

In order to achieve the proof of Theorem 2.3 we proceed as follows. First of all we establish a global existence and uniqueness result for an approximating problem. Next, we perform some a priori estimates that enable us to pass to the limit.

In this section, we approximate the system (2.24)-(2.29) by use of a semi-implicit time discretization scheme. Thus, letting N be an arbitrary positive integer, we denote by $\tau := T/N$ the time step of our backward finite differences scheme. In the forthcoming analysis, we will extensively use the following notation. Let $(V^0, V^1, ..., V^N)$ be a vector. Then, we denote by v_τ and $\bar{v}_\tau$ two functions defined on the time intervals $[0,T]$ and $(-\infty, T]$ which interpolate the values of the vector piecewise linearly and backward constantly, respectively. That is,

$$v_\tau(0) := V^0, \qquad v_\tau(t) := a_i(t)V^i + (1 - a_i(t))V^{i-1} \tag{3.1}$$

$$\bar{v}_\tau(t) := V^0 \text{ if } t \leq 0, \quad \bar{v}_\tau(t) := V^i \text{ if } t \in ((i-1)\tau, i\tau] \tag{3.2}$$

where

$$a_i(t) := \frac{(t - (i-1)\tau)}{\tau} \text{ if } t \in ((i-1)\tau, i\tau], \tag{3.3}$$

for $i = 1, ..., N$. Moreover, let us introduce the backward translation operator $\mathcal{T}_\tau$ related to the time step τ by setting

$$\begin{aligned} &\mathcal{T}_\tau f(x,t) := f(x, t-\tau) \text{ for a.e. } (x,t) \in \Omega \times (0,T), \\ &\forall f : \Omega \times (-T, T) \to \mathbb{R} \text{ measurable.} \end{aligned} \tag{3.4}$$

Next we regularize the initial datum for the internal variable p by defining

$$p_{0\tau} = \begin{cases} p_0 & \text{if } p_0 \geq \tau \\ \tau & \text{if } p_0 < \tau. \end{cases} \tag{3.5}$$

Clearly, the regularized datum $p_{0\tau}$ is still in V. Let us note that, thanks to (2.35), $\log p_{0\tau} \in L^1(\Omega)$ and moreover

$$\|p_{0\tau}\|_V + \|\log p_{0\tau}\|_{L^1(\Omega)} \leq C, \tag{3.6}$$

for some constant C depending only on $\|p_0\|_V$, $\|\log p_0\|_{L^1(\Omega)}$, $|\Omega|$ and T. Besides, in view of (2.35), (3.5) ensures that

$$\log p_{0\tau} \in H \quad \forall \tau \tag{3.7}$$

as well. Let us note in advance that, in the approximating form, we set the variational inclusion (2.27) in H by substituting the abstract operator $\partial_{V,V'} J$ by the corresponding maximal monotone graph $\partial_H J_H$ in H, provided we can prove some regularity of the solutions. As a consequence we will be able to solve the discrete variational inclusion a.e. in Ω (cf. also Remark 2.2). Then, the approximated problem can be formulated as follows.

Problem P_τ. Find vectors

$$(\Theta^0, \Theta^1, ..., \Theta^N) \in V^{N+1}, \tag{3.8}$$

$$(\boldsymbol{\chi}^0, \boldsymbol{\chi}^1, ..., \boldsymbol{\chi}^N) \in W^{N+1}, \tag{3.9}$$

$$(P^0, P^1, ..., P^N) \in V^{N+1}, \tag{3.10}$$

satisfying

$$\Theta^0 = \theta_0, \quad \boldsymbol{\chi}^0 = \chi_0, \quad P^0 = p_{0\tau}, \tag{3.11}$$

and such that, by setting

$$E^0 = \Theta^0 - \boldsymbol{\chi}^0(h(\Theta^0) - \Theta^0 h'(\Theta^0)), \tag{3.12}$$

$$U^0 = \frac{P^0}{1 + \boldsymbol{\chi}^0}, \tag{3.13}$$

the following equations hold for $i = 1, ..., N$

$$\frac{E^i - E^{i-1}}{\tau} + \mathcal{A}\Theta^i = -h(\Theta^{i-1})\frac{\boldsymbol{\chi}^i - \boldsymbol{\chi}^{i-1}}{\tau} + \left(\frac{\boldsymbol{\chi}^i - \boldsymbol{\chi}^{i-1}}{\tau}\right)^2 \quad \text{in} \quad V', \tag{3.14}$$

$$E^i = \Theta^i - \boldsymbol{\chi}^i(h(\Theta^i) - \Theta^i h'(\Theta^i)), \tag{3.15}$$

$$\frac{\boldsymbol{\chi}^i - \boldsymbol{\chi}^{i-1}}{\tau} + \nu\frac{\mathcal{A}\boldsymbol{\chi}^i - \mathcal{A}\boldsymbol{\chi}^{i-1}}{\tau} + \mathcal{A}\boldsymbol{\chi}^i + \Xi^i = h(\Theta^{i-1}) - \log P^{i-1} \quad \text{in} \quad V', \tag{3.16}$$

$$\frac{U^i - U^{i-1}}{\tau} + \mathcal{B}P^i = 0 \quad \text{in} \quad V', \tag{3.17}$$

$$U^i = \frac{P^i}{1 + \boldsymbol{\chi}^i}, \tag{3.18}$$

for

$$\Xi^i \in \partial_H J_H(\boldsymbol{\chi}^i). \tag{3.19}$$

Remark 3.1. *Since we have set the variational inclusion* (3.19) *in H and due to the regularity assumptions, we will see that equation* (3.16) *turns out to make sense also in H.*

Let us note that (3.19) implies that $\Xi^i \in \beta(\boldsymbol{\chi}^i)$ a.e. in Ω; in particular, since $D(\hat{\beta})$ is included in some bounded interval $[0, \lambda_\beta]$ (see (2.2) and (2.36)), we can infer

$$0 \le \boldsymbol{\chi}^i \le \lambda_\beta \quad \forall i = 0, ..., N, \tag{3.20}$$

a.e. in Ω. The conditions in (3.11), combined with (3.12) and (3.13), provide that (cf. (2.31)-(2.32))

$$E^0 = e_0, \tag{3.21}$$

$$U^0 = u_{0\tau} := \frac{p_{0\tau}}{1 + \chi_0}. \tag{3.22}$$

We can prove existence and uniqueness of a solution for the approximating discrete problem P_τ at any step $\tau > 0$. Indeed, the following lemma holds.

Lemma 3.2 (**Discrete well-posedness**). *Under the assumption* (2.33)-(2.35) *and* (2.39)-(2.41), *for any $\tau > 0$ the problem P_τ admits a unique solution.*

Proof. Owing to (3.11)-(3.13), (2.33)-(2.35) and (3.5), we can restrict ourselves to prove that for any fixed $\tau > 0$ and for any $i \ge 1$, the system (3.14)-(3.19) admits a unique solution. The main idea is to proceed by induction on i. Indeed, we suppose to know

$$(\Theta^{i-1}, \boldsymbol{\chi}^{i-1}, P^{i-1}) \in V \times (W \cap D(J_H)) \times V. \tag{3.23}$$

with

$$\log P^{i-1} \in H. \tag{3.24}$$

(see (3.7)). We look for

$$(\Theta^i, \boldsymbol{\chi}^i, P^i) \in V \times (W \cap D(J_H)) \times V \tag{3.25}$$

solving the resulting equations (3.14)-(3.19) and such that

$$\log P^i \in H. \tag{3.26}$$

We take first (3.16) and rewrite it as

$$\frac{\boldsymbol{\chi}^i}{\tau} + \left(1 + \frac{\nu}{\tau}\right)\mathcal{A}\boldsymbol{\chi}^i + \Xi^i = \frac{\boldsymbol{\chi}^{i-1}}{\tau} + \frac{\nu}{\tau}\mathcal{A}\boldsymbol{\chi}^{i-1} + h(\Theta^{i-1}) - \log P^{i-1}. \tag{3.27}$$

Since we are assuming (2.39)-(2.40) and (3.23)-(3.24) we can observe that the right hand side, say $\mathcal{F}$, is known in H. Thus relation (3.27) can be equivalently rewritten as

$$(\tau^{-1}Id + \mathcal{C} + \partial_H J_H)\boldsymbol{\chi}^i \ni \mathcal{F}, \tag{3.28}$$

where

$$\mathcal{C}\boldsymbol{\chi}^i = (1 + \nu\tau^{-1})\mathcal{A}\boldsymbol{\chi}^i.$$

Actually, we would like to exploit the well known results on the maximality of sums of monotone operators, holding under particular regularity conditions. Namely, in this framework, we can invoke Theorem 7.2 and get the required existence of a function $\boldsymbol{\chi}^i \in W \cap D(J_H)$ fulfilling (3.16). On a second step, we take into consideration (3.17), where $\boldsymbol{\chi}^i$ is now the solution of (3.16). Equation (3.17) can be reformulated as follows

$$\tau^{-1}\frac{P^i}{1+\boldsymbol{\chi}^i} + \mathcal{B}P^i = \tau^{-1}\frac{P^{i-1}}{1+\boldsymbol{\chi}^{i-1}} \tag{3.29}$$

The existence and uniqueness of a solution $P^i \in V$ follows directly from the Lax-Milgram theorem, taking into account that $\boldsymbol{\chi}^i$ satisfies (3.20). Before proceeding, we have to check that (3.26) holds. To this aim, we refer to the First a priori estimate, where we will prove that $\log U^i \in V$ (see (4.23)). In particular, this and the fact that $\boldsymbol{\chi}^i$ obeys (3.20) yield (3.26). Namely, owing to (3.18), there is a constant C such that

$$\left\|\log P^i\right\|_H \le C\left(\left\|\log U^i\right\|_H + \left\|\boldsymbol{\chi}^i\right\|_H\right). \tag{3.30}$$

Finally, letting in (3.14) $\boldsymbol{\chi}^i$ be the unique solution of (3.16) and exploiting once more standard results on maximal monotone operators we can find a unique function $\Theta^i \in V$ solving the equation. Indeed we can rewrite (3.14) more explicitly in terms of Θ^i as

$$\begin{aligned} &\tau^{-1}\Theta^i - \tau^{-1}\boldsymbol{\chi}^i(h(\Theta^i) - \Theta^i h'(\Theta^i)) + \mathcal{A}\Theta^i \\ &= \tau^{-1}\Theta^{i-1}(1 + h'(\Theta^{i-1})\boldsymbol{\chi}^{i-1}) - \tau^{-1}h(\Theta^{i-1})\boldsymbol{\chi}^i + \left(\frac{\boldsymbol{\chi}^i - \boldsymbol{\chi}^{i-1}}{\tau}\right)^2. \end{aligned} \tag{3.31}$$

As the right hand side, say $\mathcal{G}$, is known in H the above relation can be equivalently rewritten as

$$(\tau^{-1}(Id + \mathcal{R}_i) + \mathcal{A})\Theta^i \ni \mathcal{G}, \tag{3.32}$$

where Id stands for the identity operator in H and

$$\mathcal{R}_i(\Theta^i) = \boldsymbol{\chi}^i(\Theta^i h'(\Theta^i) - h(\Theta^i))$$

maps H into H. For the sake of clarity, in our notation the subscript i in $\mathcal{R}_i$ is used for pointing out the dependence of $\mathcal{R}_i$ on $\boldsymbol{\chi}^i$. Then, in view of assumptions (2.40)-(2.41) it is not difficult to check that $Id + \mathcal{R}_i$ is a Lipschitz continuous and strongly monotone operator from H into H, and consequently coercive. Since $\mathcal{A}$ is a maximal monotone operator with domain W, the hypotheses of, e.g., [3, Cor 1.3, p. 48] hold and we get the required existence and uniqueness of a solution $\Theta^i \in V$ to equation (3.14). This concludes our proof of Lemma 3.2, since for any i, and any fixed $\tau > 0$, the corresponding triple $(\Theta^i, \boldsymbol{\chi}^i, P^i)$ solves the system (3.14)-(3.19). □

4. A priori estimates

In this section, we aim to establish some a priori estimates on the time-discrete solutions whose existence has been proved in Lemma 3.2. By virtue of Lemma 3.2 and owing to the position (3.1)-(3.4), we may introduce the piecewise constant and linear in time functions $\bar\theta_\tau$, $\bar e_\tau$, $\bar\chi_\tau$, $\bar\xi_\tau$, $\bar p_\tau$, $\bar u_\tau$, θ_τ, e_τ, χ_τ, p_τ, u_τ interpolating the corresponding values. Thanks to these notations, the scheme (3.14)-(3.18) is restated as follows in V' and a.e. in $(0,T)$

$$\partial_t e_\tau + \mathcal{A}\bar\theta_\tau = -h(\mathcal{T}_\tau\bar\theta_\tau)\partial_t\chi_\tau + (\partial_t\chi_\tau)^2, \tag{4.1}$$

$$\bar e_\tau = \bar\theta_\tau - \bar\chi_\tau(h(\bar\theta_\tau) - \bar\theta_\tau h'(\bar\theta_\tau)), \tag{4.2}$$

$$\partial_t\chi_\tau + \nu\mathcal{A}(\partial_t\chi_\tau) + \mathcal{A}\bar\chi_\tau + \bar\xi_\tau = h(\mathcal{T}_\tau\bar\theta_\tau) - \mathcal{T}_\tau(\log\bar p_\tau), \tag{4.3}$$

$$\bar\xi_\tau \in \partial_{V,V'}J(\bar\chi_\tau), \tag{4.4}$$

$$\partial_t u_\tau + \mathcal{B}\bar p_\tau = 0, \tag{4.5}$$

$$\bar u_\tau = \frac{\bar p_\tau}{1+\bar\chi_\tau}. \tag{4.6}$$

As concerns the inclusion (3.16) we could write it in H in terms of the above introduced piecewise linear and constant functions. Nonetheless, in order to perform a passage to the limit procedure as $\tau \searrow 0$, we have to set this inclusion in the abstract framework of the $V - V'$ duality. Thus, instead of $\partial_H J_H$ we have written the corresponding abstract operator $\partial_{V,V'}J$ in (4.4). Obviously, by the regularity of the solution vectors, the existence and uniqueness result we have proved in the previous section can be extended to the abstract framework of V'. In addition, let us observe that by construction (cf. (3.1)), χ_τ, θ_τ, p_τ, e_τ and u_τ satisfy the natural Cauchy conditions (cf. (3.5), (3.11) and (3.21)-(3.22))

$$\chi_\tau(0) = \chi_0, \tag{4.7}$$
$$\theta_\tau(0) = \theta_0, \tag{4.8}$$
$$p_\tau(0) = p_{0\tau}, \tag{4.9}$$
$$e_\tau(0) = e_0, \tag{4.10}$$
$$u_\tau(0) = u_{0\tau}. \tag{4.11}$$

Hence, we are going to prove some estimates on the approximating functions solving (4.1)-(4.6); such estimates hold at least for τ sufficiently small, but the involved constants do not depend on τ. Indeed, our aim is passing to the limit in the above system as $\tau \searrow 0$, by compactness or direct proof, to get (2.24)-(2.29) solved in a suitable sense. Let us recall the trivial equality

$$2a(a-b) = a^2 + (a-b)^2 - b^2, \quad \forall a, b \in \mathbb{R}, \tag{4.12}$$

which will be applied in the following estimates on the discrete solutions.

First a priori estimate. We first test equation (3.16) by $(\boldsymbol{\chi}^i - \chi_*)$, where the value χ_* is introduced in (2.3) and satisfies $0 \in \beta(\chi_*)$. Let us observe that, by monotonicity of the operator $\partial_H J_H$, (3.19) yields

$$\int_\Omega \Xi^i(\boldsymbol{\chi}^i - \chi_*) \geq 0. \tag{4.13}$$

Hence, exploiting the relation (4.12), by using (4.13), we get

$$\begin{aligned}
&\frac{1}{2\tau}\left\|\boldsymbol{\chi}^i - \chi_*\right\|_H^2 + \frac{1}{2\tau}\left\|\boldsymbol{\chi}^i - \boldsymbol{\chi}^{i-1}\right\|_H^2 - \frac{1}{2\tau}\left\|\boldsymbol{\chi}^{i-1} - \chi_*\right\|_H^2 + \left(1 + \frac{\nu}{2\tau}\right)\left\|\nabla\boldsymbol{\chi}^i\right\|_H^2 \\
&+ \frac{\nu}{2\tau}\left\|\nabla\boldsymbol{\chi}^i - \nabla\boldsymbol{\chi}^{i-1}\right\|_H^2 - \frac{\nu}{2\tau}\left\|\nabla\boldsymbol{\chi}^{i-1}\right\|_H^2 \\
&\leq \int_\Omega h(\Theta^{i-1})(\boldsymbol{\chi}^i - \chi_*) - \int_\Omega \log P^{i-1}(\boldsymbol{\chi}^i - \chi_*).
\end{aligned} \tag{4.14}$$

Then, we would like to formally test equation (3.17) by $1 - 1/U^i$. Nevertheless, in order to make the desired estimate rigorous we perform a detailed procedure. Thus, let $0 < \varepsilon < 1$ and $\gamma_\varepsilon(\cdot)$ be defined by

$$\gamma_\varepsilon(s) := \begin{cases} 1 - \dfrac{1}{s} & \text{if } s \geq \varepsilon \\ 1 - \dfrac{1}{\varepsilon} & \text{if } s < \varepsilon \end{cases} \tag{4.15}$$

Next, we introduce the primitive function Γ_ε defined by

$$\Gamma_\varepsilon(u) = \int_1^u \gamma_\varepsilon(s)ds + 1, \tag{4.16}$$

so that it results

$$\begin{aligned}
&\Gamma_\varepsilon(u) = u - \log u \quad \text{if } u \geq \varepsilon \\
&\Gamma_\varepsilon(u) = 1 + \log\frac{1}{\varepsilon} + \left(1 - \frac{1}{\varepsilon}\right)u \quad \text{if } u < \varepsilon.
\end{aligned} \tag{4.17}$$

Now, we rewrite (3.17) in terms of the variables $\boldsymbol{\chi}^i$ and U^i thus obtaining

$$\frac{U^i - U^{i-1}}{\tau} + \mathcal{B}(U^i(1 + \boldsymbol{\chi}^i)) = 0. \tag{4.18}$$

Hence, we test (4.18) by $\gamma_\varepsilon(U^i)$ and, thanks to the convexity of Γ_ε, we obtain

$$\begin{aligned}
&\frac{1}{\tau}\int_\Omega \Gamma_\varepsilon(U^i) - \frac{1}{\tau}\int_\Omega \Gamma_\varepsilon(U^{i-1}) + \int_\Omega \left|\nabla U^i\right|^2 (1 + \boldsymbol{\chi}^i)\gamma_\varepsilon'(U^i) \\
&+ \int_\Omega U^i \nabla U^i \nabla \boldsymbol{\chi}^i \gamma_\varepsilon'(U^i) + \int_\Gamma U^i(1 + \boldsymbol{\chi}^i)\gamma_\varepsilon(U^i) \leq 0.
\end{aligned} \tag{4.19}$$

By virtue of (4.15), (4.19) yields

$$\begin{aligned}&\frac{1}{\tau}\int_\Omega \Gamma_\varepsilon(U^i)+\int_{\Omega\cap\{U^i\geq\varepsilon\}}\left|\nabla\log U^i\right|^2(1+\boldsymbol{\chi}^i)+\int_{\Gamma\cap\{U^i\geq 0\}}U^i\\&\leq\frac{1}{\tau}\int_\Omega\Gamma_\varepsilon(U^{i-1})+\int_{\Gamma\cap\{U^i\geq 0\}}(1+\boldsymbol{\chi}^i)-\int_{\Omega\cap\{U^i\geq\varepsilon\}}\nabla\log U^i\nabla\boldsymbol{\chi}^i.\end{aligned}\tag{4.20}$$

The second integral on the right hand side turns out to be uniformly bounded thanks to (3.20), while we can exploit the Young inequality in order to treat the last term of (4.20). Eventually, using once more (3.20), from (4.20) we can obtain

$$\begin{aligned}&\frac{1}{\tau}\int_\Omega \Gamma_\varepsilon(U^i)+\frac{1}{2}\int_{\Omega\cap\{U^i\geq\varepsilon\}}\left|\nabla\log U^i\right|^2+\int_{\Gamma\cap\{U^i\geq 0\}}U^i\\&\leq C_0+\frac{1}{\tau}\int_\Omega\Gamma_\varepsilon(U^{i-1})+\frac{1}{2}\int_\Omega\left|\nabla\boldsymbol{\chi}^i\right|^2.\end{aligned}\tag{4.21}$$

where C_0 depends on λ_β. Let us note that, by inductive hypothesis, we are assuming $\log P^{i-1}\in H$, which implies $\log U^{i-1}\in H$ (see (3.18)), whence $U^{i-1}>0$ a.e. in Ω. Analogously, since $P^{i-1}\in V$ and (3.20) holds, we have also that $U^{i-1}\in H$. In particular, we can infer that $\left(U^{i-1}-\log U^{i-1}\right)\in L^1(\Omega)$. Finally, we observe that the last integral on the right hand side of (4.21) is bounded thanks to the regularity of $\boldsymbol{\chi}^i$ ($\boldsymbol{\chi}^i\in W$). Thus, to pass to the limit as $\varepsilon\searrow 0$ in (4.21), we can apply the monotone convergence theorem and get

$$\begin{aligned}&\frac{1}{\tau}\int_\Omega(U^i-\log U^i)+\frac{1}{2}\int_\Omega\left|\nabla\log U^i\right|^2+\int_\Gamma U^i\\&\leq C_0+\frac{1}{\tau}\int_\Omega(U^{i-1}-\log U^{i-1})+\frac{1}{2}\int_\Omega\left|\nabla\boldsymbol{\chi}^i\right|^2.\end{aligned}\tag{4.22}$$

Due to the previous estimates and to the Poincaré-Wirtinger inequality, from (4.22) we infer

$$(U^i-\log U^i)\in L^1(\Omega)\quad\text{and}\quad\log U^i\in V,\tag{4.23}$$

whence $U^i>0$ a.e. in Ω. Now, we combine the estimates (4.14) and (4.22) and sum them. By use of (3.18) we easily deduce

$$\begin{aligned}&\frac{1}{2\tau}\left\|\boldsymbol{\chi}^i-\chi_*\right\|_H^2+\frac{1}{2\tau}\left\|\boldsymbol{\chi}^i-\boldsymbol{\chi}^{i-1}\right\|_H^2-\frac{1}{2\tau}\left\|\boldsymbol{\chi}^{i-1}-\chi_*\right\|_H^2\\&+\left(\frac{1}{2}+\frac{\nu}{2\tau}\right)\left\|\nabla\boldsymbol{\chi}^i\right\|_H^2+\frac{\nu}{2\tau}\left\|\nabla\boldsymbol{\chi}^i-\nabla\boldsymbol{\chi}^{i-1}\right\|_H^2-\frac{\nu}{2\tau}\left\|\nabla\boldsymbol{\chi}^{i-1}\right\|_H^2\\&+\frac{1}{\tau}\int_\Omega(U^i-\log U^i)+\frac{1}{2}\int_\Omega\left|\nabla\log U^i\right|^2+\int_\Gamma U^i\\&+\int_\Omega\log(1+\boldsymbol{\chi}^{i-1})\boldsymbol{\chi}^i\leq C_0+\frac{1}{\tau}\int_\Omega(U^{i-1}-\log U^{i-1})\\&+\int_\Omega h(\Theta^{i-1})(\boldsymbol{\chi}^i-\chi_*)-\int_\Omega\log U^{i-1}(\boldsymbol{\chi}^i-\chi_*)+\int_\Omega\log(1+\boldsymbol{\chi}^{i-1})\chi_*.\end{aligned}\tag{4.24}$$

Let us observe that the last integral on the left hand side is non-negative (see (3.20)). Besides, owing to (3.20), we can handle the last integral on the right hand side of (4.24) as follows

$$\int_\Omega\log(1+\boldsymbol{\chi}^{i-1})\chi_*\leq\int_\Omega\boldsymbol{\chi}^{i-1}\chi_*\leq\lambda_\beta^2\left|\Omega\right|.\tag{4.25}$$

Hence, by summing up (4.24) for $i = 1, \dots\dots, m$, with $m \leq N = T/\tau$, and multiplying by τ, we obtain

$$\begin{aligned}
&\frac{1}{2}\left\|\boldsymbol{\chi}^m - \chi_*\right\|_H^2 + \frac{1}{2}\sum_{i=1}^m \tau\left\|\nabla\boldsymbol{\chi}^i\right\|_H^2 + \frac{\nu}{2}\left\|\nabla\boldsymbol{\chi}^m\right\|_H^2 \\
&+ \int_\Omega (U^m - \log U^m) + \frac{1}{2}\sum_{i=1}^m \tau \int_\Omega \left|\nabla \log U^i\right|^2 + \sum_{i=1}^m \tau \int_\Gamma U^i \\
&\leq \tilde{C}_0 + \frac{1}{2}\left\|\boldsymbol{\chi}^0 - \chi_*\right\|_H^2 + \frac{\nu}{2}\left\|\nabla\boldsymbol{\chi}^0\right\|_H^2 + \int_\Omega (U^0 - \log U^0) \\
&+ \sum_{i=1}^m \tau \int_\Omega h(\Theta^{i-1})(\boldsymbol{\chi}^i - \chi_*) - \sum_{i=1}^m \tau \int_\Omega \log U^{i-1}(\boldsymbol{\chi}^i - \chi_*),
\end{aligned} \tag{4.26}$$

where $\tilde{C_0} = (C_0 + \lambda_\beta^2\,|\Omega|)T$. Now, owing to (2.39) and (3.20), by use of the Hölder and Young inequalities we can find two positive constants C_1 and C_2 such that the following estimate holds

$$\begin{aligned}
&\frac{1}{2}\left\|\boldsymbol{\chi}^m - \chi_*\right\|_H^2 + \frac{1}{2}\sum_{i=1}^m \tau\left\|\nabla\boldsymbol{\chi}^i\right\|_H^2 + \frac{\nu}{2}\left\|\nabla\boldsymbol{\chi}^m\right\|_H^2 \\
&+ \int_\Omega (U^m - \log U^m) + \frac{1}{2}\sum_{i=1}^m \tau \int_\Omega \left|\nabla \log U^i\right|^2 + \sum_{i=1}^m \tau \int_\Gamma U^i \\
&\leq C_1 + \frac{1}{2}\left\|\boldsymbol{\chi}^0 - \chi_*\right\|_H^2 + \frac{\nu}{2}\left\|\nabla\boldsymbol{\chi}^0\right\|_H^2 \\
&+ \int_\Omega U^0 + C_2\int_\Omega \left|\log U^0\right| + 2\lambda_\beta \sum_{i=1}^{m-1} \tau \left\|\log U^i\right\|_{L^1(\Omega)}.
\end{aligned} \tag{4.27}$$

Let us remind that $U^0 = u_{0\tau} = p_{0\tau}/(1+\chi_0)$ and $\log U^0 = \log u_{0\tau} = \log p_{0\tau} - \log(1+\chi_0)$. Then, in virtue of (2.36) and (3.6) we can write

$$\begin{aligned}
&\frac{1}{2}\left\|\boldsymbol{\chi}^m - \chi_*\right\|_H^2 + \frac{1}{2}\sum_{i=1}^m \tau\left\|\nabla\boldsymbol{\chi}^i\right\|_H^2 + \frac{\nu}{2}\left\|\nabla\boldsymbol{\chi}^m\right\|_H^2 \\
&+ \int_\Omega (U^m - \log U^m) + \frac{1}{2}\sum_{i=1}^m \tau \int_\Omega \left|\nabla \log U^i\right|^2 + \sum_{i=1}^m \tau \int_\Gamma U^i \\
&\leq C_3 + \frac{1}{2}\left\|\boldsymbol{\chi}^0 - \chi_*\right\|_H^2 + \frac{\nu}{2}\left\|\nabla\boldsymbol{\chi}^0\right\|_H^2 + 2\lambda_\beta \sum_{i=1}^{m-1} \tau \left\|\log U^i\right\|_{L^1(\Omega)},
\end{aligned} \tag{4.28}$$

for some positive constant C_3 not depending on τ. Moreover, let us note that the following inequality holds

$$\frac{1}{3}(U^i + \left|\log U^i\right|) \leq (U^i - \log U^i). \tag{4.29}$$

As a consequence of (4.29) and owing to (3.11) we can finally obtain

$$\begin{aligned}
&\frac{1}{2}\left\|\boldsymbol{\chi}^m - \chi_*\right\|_H^2 + \frac{1}{2}\sum_{i=1}^m \tau\left\|\nabla\boldsymbol{\chi}^i\right\|_H^2 + \frac{\nu}{2}\left\|\nabla\boldsymbol{\chi}^m\right\|_H^2 \\
&+ \frac{1}{3}\left\|U^m\right\|_{L^1(\Omega)} + \frac{1}{3}\left\|\log U^m\right\|_{L^1(\Omega)} + \frac{1}{2}\sum_{i=1}^m \tau \int_\Omega \left|\nabla \log U^i\right|^2 + \sum_{i=1}^m \tau \int_\Gamma U^i \\
&\leq C_3 + \frac{1}{2}\left\|\chi_0 - \chi_*\right\|_H^2 + \frac{\nu}{2}\left\|\nabla\chi_0\right\|_H^2 + 2\lambda_\beta \sum_{i=1}^{m-1} \tau \left\|\log U^i\right\|_{L^1(\Omega)}.
\end{aligned} \tag{4.30}$$

Thus, the Poincaré inequality and the discrete Gronwall lemma [14, Prop. 2.2.1] applied to (4.30) imply (see (2.34) and (2.36))

$$\begin{aligned}
&\left\|\bar{\chi}_\tau\right\|_{L^\infty(0,T,V)} + \left\|\bar{u}_\tau\right\|_{L^\infty(0,T,L^1(\Omega))} \\
&+ \left\|\bar{u}_\tau|_\Gamma\right\|_{L^1(0,T,L^1(\Gamma))} + \left\|\log \bar{u}_\tau\right\|_{L^\infty(0,T,L^1(\Omega)) \cap L^2(0,T,V)} \leq C.
\end{aligned} \tag{4.31}$$

In particular, note that $\bar{u}_\tau > 0$ almost everywhere in Q.

Second a priori estimate. From the estimates on $\bar{u}_\tau$ in (4.31) it is possible to deduce analogous regularities for $\bar{p}_\tau = \bar{u}_\tau(1+\bar{\chi}_\tau)$. In particular, let us discuss the regularity of $\log \bar{p}_\tau$. Since (3.20) holds, we can infer that $\bar{\chi}_\tau \geq 0$ a.e. in Q and $\bar{\chi}_\tau \in L^\infty(Q)$ (see (2.23) and (2.2)). Hence, thanks to (4.6), we have that

$$\begin{aligned}&\|\log \bar{p}_\tau\|_{L^\infty(0,T,L^1(\Omega))\cap L^2(0,T,V)} \\ &\leq C_4 \left(\|\log \bar{u}_\tau\|_{L^\infty(0,T,L^1(\Omega))\cap L^2(0,T,V)} + \|\bar{\chi}_\tau\|_{L^\infty(0,T,L^1(\Omega))\cap L^2(0,T,V)} \right) \leq C. \end{aligned} \tag{4.32}$$

Third a priori estimate. We test (3.16) by $\boldsymbol{\chi}^i - \boldsymbol{\chi}^{i-1}$. Thanks to (4.12) and (3.19), we get

$$\begin{aligned}&\tau \left\| \frac{\boldsymbol{\chi}^i - \boldsymbol{\chi}^{i-1}}{\tau} \right\|_H^2 + \nu\tau \left\| \frac{\nabla(\boldsymbol{\chi}^i - \boldsymbol{\chi}^{i-1})}{\tau} \right\|_H^2 + \frac{1}{2} \|\nabla \boldsymbol{\chi}^i\|_H^2 \\ &+ \frac{\tau^2}{2} \left\| \frac{\nabla(\boldsymbol{\chi}^i - \boldsymbol{\chi}^{i-1})}{\tau} \right\|_H^2 - \frac{1}{2} \|\nabla \boldsymbol{\chi}^{i-1}\|_H^2 + \int_\Omega \hat{\beta}(\boldsymbol{\chi}^i) - \int_\Omega \hat{\beta}(\boldsymbol{\chi}^{i-1}) \\ &\leq \int_\Omega (\boldsymbol{\chi}^i - \boldsymbol{\chi}^{i-1})(h(\Theta^{i-1}) - \log P^{i-1}). \end{aligned} \tag{4.33}$$

Now, we can handle the integral on the right hand side of (4.33) by means of the Young inequality and get

$$\begin{aligned}&\int_\Omega (\boldsymbol{\chi}^i - \boldsymbol{\chi}^{i-1})(h(\Theta^{i-1}) - \log P^{i-1}) \\ &\leq \frac{\tau}{2} \left\| \frac{\boldsymbol{\chi}^i - \boldsymbol{\chi}^{i-1}}{\tau} \right\|_H^2 + \frac{\tau}{2} \left(|\Omega| \, \|h\|_{L^\infty(\mathbb{R})}^2 + \left\|\log P^{i-1}\right\|_H^2 \right). \end{aligned} \tag{4.34}$$

Thus, we add (4.33) for $i = 1, ..., m$, with $m \leq N$ and we easily recover (cf. (2.40), (3.11) and (4.32))

$$\begin{aligned}&\frac{1}{2} \sum_{i=1}^m \tau \left\| \frac{\boldsymbol{\chi}^i - \boldsymbol{\chi}^{i-1}}{\tau} \right\|_H^2 + \nu \sum_{i=1}^m \tau \left\| \frac{\nabla(\boldsymbol{\chi}^i - \boldsymbol{\chi}^{i-1})}{\tau} \right\|_H^2 + \frac{1}{2} \|\nabla \boldsymbol{\chi}^m\|_H^2 \\ &+ \int_\Omega \hat{\beta}(\boldsymbol{\chi}^m) \leq C_5 + \frac{1}{2} \|\nabla \chi_0\|_H^2 + \int_\Omega \hat{\beta}(\chi_0). \end{aligned} \tag{4.35}$$

Hence, owing to (2.34), we obtain the following bound

$$\|\chi_\tau\|_{H^1(0,T;V)} + \left\| \hat{\beta}(\bar{\chi}_\tau) \right\|_{L^\infty(0,T;L^1(\Omega))} \leq C. \tag{4.36}$$

Fourth a priori estimate. We proceed by formally testing (3.16) by $\tau \mathcal{A} \boldsymbol{\chi}^i$. Due to the monotonicity of the operator $\partial_H J_H$, it turns out that $\tau \int_\Omega \Xi^i \mathcal{A} \boldsymbol{\chi}^i \geq 0$. Hence, by exploiting once more (4.12) and Young's inequality, by similarly proceeding as for (4.33), we owe to (2.40), (4.31) and write

$$\begin{aligned}&\frac{1}{2} \|\nabla \boldsymbol{\chi}^i\|_H^2 - \frac{1}{2} \|\nabla \boldsymbol{\chi}^{i-1}\|_H^2 + \frac{1}{2} \|\mathcal{A} \boldsymbol{\chi}^i\|_H^2 - \frac{1}{2} \|\mathcal{A} \boldsymbol{\chi}^{i-1}\|_H^2 + \tau \|\mathcal{A} \boldsymbol{\chi}^i\|_H^2 \\ &\leq \frac{\tau}{2} \|\mathcal{A} \boldsymbol{\chi}^i\|_H^2 + \frac{\tau}{2} \left(|\Omega| \, \|h\|_{L^\infty(\mathbb{R})}^2 + \left\|\log P^{i-1}\right\|_H^2 \right). \end{aligned} \tag{4.37}$$

If we sum up in (4.37) for $i = 1, ..., m$, we get (see (2.40), (3.11) and (4.32))

$$\|\nabla \boldsymbol{\chi}^m\|_H^2 + \|\mathcal{A} \boldsymbol{\chi}^m\|_H^2 + \sum_{i=1}^m \tau \|\mathcal{A} \boldsymbol{\chi}^i\|_H^2 \leq \|\nabla \chi_0\|_H^2 + \|\mathcal{A} \chi_0\|_H^2 + C_6, \tag{4.38}$$

for any $m \leq N$. Finally, the regularity assumptions (2.34) on χ_0 ensure that

$$\|\bar{\chi}_\tau\|_{L^\infty(0,T,W)} \leq C. \tag{4.39}$$

Fifth a priori estimate. Test equation (3.14) by E^i. Exploiting once more (4.12) and recalling that $E^i = \psi(\Theta^i, \boldsymbol{\chi}^i)$ (see (3.15)), we can write

$$\begin{aligned}
&\frac{1}{2\tau}\left\|E^i\right\|_H^2 + \frac{1}{2\tau}\left\|E^i - E^{i-1}\right\|_H^2 - \frac{1}{2\tau}\left\|E^{i-1}\right\|_H^2 \\
&+ \int_\Omega \left|\nabla\Theta^i\right|^2 \partial_1\psi(\Theta^i, \boldsymbol{\chi}^i) + \int_\Omega \nabla\Theta^i \nabla\boldsymbol{\chi}^i \partial_2\psi(\Theta^i, \boldsymbol{\chi}^i) \\
&= -\int_\Omega h(\Theta^{i-1}) E^i \frac{\boldsymbol{\chi}^i - \boldsymbol{\chi}^{i-1}}{\tau} + \int_\Omega E^i \left(\frac{\boldsymbol{\chi}^i - \boldsymbol{\chi}^{i-1}}{\tau}\right)^2. \qquad (4.40)
\end{aligned}$$

To handle the last integral on the right-hand side we use the extended Hölder inequality and get

$$\int_\Omega E^i \left(\frac{\boldsymbol{\chi}^i - \boldsymbol{\chi}^{i-1}}{\tau}\right)^2 \leq \left\|E^i\right\|_H \left\|\frac{\boldsymbol{\chi}^i - \boldsymbol{\chi}^{i-1}}{\tau}\right\|_{L^4(\Omega)}^2. \qquad (4.41)$$

We recall the bounds on $\partial_1\psi$ and $|\partial_2\psi|$ stated in (2.42)-(2.43). Then, due to (2.40), (4.41) and the Young and Hölder inequalities, we can infer

$$\begin{aligned}
&\frac{1}{2\tau}\left\|E^i\right\|_H^2 + \frac{\tau}{2}\left\|\frac{E^i - E^{i-1}}{\tau}\right\|_H^2 - \frac{1}{2\tau}\left\|E^{i-1}\right\|_H^2 + \frac{c_s}{2}\left\|\nabla\Theta^i\right\|_H^2 \\
&\leq C_7\left\|\nabla\boldsymbol{\chi}^i\right\|_H^2 + c_h\left\|E^i\right\|_H \left\|\frac{\boldsymbol{\chi}^i - \boldsymbol{\chi}^{i-1}}{\tau}\right\|_H + \left\|E^i\right\|_H \left\|\frac{\boldsymbol{\chi}^i - \boldsymbol{\chi}^{i-1}}{\tau}\right\|_{L^4(\Omega)}^2, \qquad (4.42)
\end{aligned}$$

where $C_7 = c_h^2/(2c_s)$. Then, multiplying (4.42) by τ and summing up for $i = 1, ..., m$, we get

$$\begin{aligned}
&\frac{1}{2}\left\|E^m\right\|_H^2 + \frac{c_s}{2}\sum_{i=1}^m \tau\left\|\nabla\Theta^i\right\|_H^2 \leq \frac{1}{2}\left\|E^0\right\|_H^2 + C_7\sum_{i=1}^m \tau\left\|\nabla\boldsymbol{\chi}^i\right\|_H^2 \\
&+ \sum_{i=1}^m \left\|E^i\right\|_H \left(c_h\tau\left\|\frac{\boldsymbol{\chi}^i - \boldsymbol{\chi}^{i-1}}{\tau}\right\|_H + \tau\left\|\frac{\boldsymbol{\chi}^i - \boldsymbol{\chi}^{i-1}}{\tau}\right\|_{L^4(\Omega)}^2\right). \qquad (4.43)
\end{aligned}$$

In order to apply the discrete Gronwall lemma [14, Prop. 2.2.1], we have to treat the m-th term in the last summation of (4.43) separately. Here, we sketch out such a procedure. Namely, we deal with the m-th term by use of the Young inequality and get

$$\begin{aligned}
&\left\|E^m\right\|_H \left(c_h\tau\left\|\frac{\boldsymbol{\chi}^m - \boldsymbol{\chi}^{m-1}}{\tau}\right\|_H + \tau\left\|\frac{\boldsymbol{\chi}^m - \boldsymbol{\chi}^{m-1}}{\tau}\right\|_{L^4(\Omega)}^2\right) \\
&\leq \frac{1}{4}\left\|E^m\right\|_H^2 + 2\tau c_h^2\left\|\partial_t\chi_\tau\right\|_{L^2(0,T,H)}^2 + 2\left\|\partial_t\chi_\tau\right\|_{L^2(0,T,L^4(\Omega))}^4. \qquad (4.44)
\end{aligned}$$

Finally, thanks to the Third estimate (see (4.36)) and to the continuous embedding $V \subset L^4(\Omega)$, we conclude that there exists a positive constant C_8 such that

$$\left\|E^m\right\|_H \left(c_h\tau\left\|\frac{\boldsymbol{\chi}^m - \boldsymbol{\chi}^{m-1}}{\tau}\right\|_H + \tau\left\|\frac{\boldsymbol{\chi}^m - \boldsymbol{\chi}^{m-1}}{\tau}\right\|_{L^4(\Omega)}^2\right) \leq C_8 + \frac{1}{4}\left\|E^m\right\|_H^2. \qquad (4.45)$$

Owing to (3.21), (4.31) and (4.45), (4.43) yields

$$\begin{aligned}
&\frac{1}{4}\left\|E^m\right\|_H^2 + \frac{c_s}{2}\sum_{i=1}^m \tau\left\|\nabla\Theta^i\right\|_H^2 \leq C_9 + \frac{1}{2}\left\|e_0\right\|_H^2 \\
&+ \sum_{i=1}^{m-1} \tau\left\|E^i\right\|_H \left(\frac{c_h^2}{2} + \frac{1}{2}\left\|\frac{\boldsymbol{\chi}^i - \boldsymbol{\chi}^{i-1}}{\tau}\right\|_H^2 + \left\|\frac{\boldsymbol{\chi}^i - \boldsymbol{\chi}^{i-1}}{\tau}\right\|_{L^4(\Omega)}^2\right). \qquad (4.46)
\end{aligned}$$

Eventually, (2.44) and (4.31)-(4.36) allow us to make use of the discrete Gronwall lemma [14, Prop. 2.2.1], thus obtaining

$$\left\|\bar{e}_\tau\right\|_{L^\infty(0,T,H)} + \left\|\nabla\bar{\theta}_\tau\right\|_{L^2(0,T,H)} \leq C. \qquad (4.47)$$

We recall that $\bar{e}_\tau$ is defined as $\bar{e}_\tau = \psi(\bar{\theta}_\tau, \bar{\chi}_\tau)$ (see (4.2)). Thus, the relation between $\bar{\theta}_\tau$ and $\bar{e}_\tau$ is bi-lipschitz (cf. (2.42)-(2.43)) and allows us to infer from (4.47) that

$$\left\|\bar{\theta}_\tau\right\|_{L^\infty(0,T,H)\cap L^2(0,T,V)} \leq C. \qquad (4.48)$$

Sixth a priori estimate. Here, we aim at deriving some further regularities for the variables e_τ and $\bar{e}_\tau$ from the previous estimates. At first, let us observe that (4.48), combined with (2.42)-(2.43) and with the regularity of $\bar{\chi}_\tau$ (see (4.31)), yields

$$\|\bar{e}_\tau\|_{L^2(0,T,V)} \le C \tag{4.49}$$

Indeed, since $\bar{e}_\tau = \psi(\bar{\theta}_\tau, \bar{\chi}_\tau)$, the following inequalities hold

$$\begin{aligned} \|\bar{e}_\tau\|^2_{L^2(0,T,V)} &= \int_0^T \|\bar{e}_\tau\|^2_H + \int_0^T \left\|\nabla\bar{\theta}_\tau \partial_1\psi(\bar{\theta}_\tau, \bar{\chi}_\tau) + \nabla\bar{\chi}_\tau\partial_2\psi(\bar{\theta}_\tau, \bar{\chi}_\tau)\right\|^2_H \\ &\le T\|\bar{e}_\tau\|^2_{L^\infty(0,T,H)} + C_e\left\|\nabla\bar{\theta}_\tau\right\|^2_{L^2(0,T,H)} + c_h^2\|\nabla\bar{\chi}_\tau\|_{L^2(0,T,H)} \le C, \end{aligned} \tag{4.50}$$

where C_e depends on c_e (see (2.42)). Moreover, from (4.49) and (2.44) we can also deduce that

$$\|e_\tau\|_{L^2(0,T,V)} \le C. \tag{4.51}$$

Finally, let us observe that (4.48) yields

$$\left\|\mathcal{A}\bar{\theta}_\tau\right\|_{L^2(0,T,V')} \le C. \tag{4.52}$$

In addition, from (4.36) we can easily deduce that

$$\left\|(\partial_t\chi_\tau)^2\right\|_{L^1(0,T,H)} \quad \text{and} \quad \left\|h(\mathcal{T}_\tau\bar{\theta}_\tau)\partial_t\chi_\tau\right\|_{L^2(0,T,H)} \le C. \tag{4.53}$$

Thus, by a comparison in (4.1), we can infer that

$$\|\partial_t e_\tau\|_{L^1(0,T,V')} \le C. \tag{4.54}$$

Seventh a priori estimate. We consider (3.17) and we rewrite it in terms of P^i, P^{i-1} and $\boldsymbol{\chi}^i$, $\boldsymbol{\chi}^{i-1}$, thus obtaining

$$\tau^{-1}\frac{P^i}{1+\boldsymbol{\chi}^i} - \tau^{-1}\frac{P^{i-1}}{1+\boldsymbol{\chi}^{i-1}} + \mathcal{B}P^i = 0. \tag{4.55}$$

Now, we test (4.55) by P^i. Thanks to (3.20), there exists a positive constant $C_\chi = 1/(1+\lambda_\beta)$ such that

$$C_\chi \le \frac{1}{1+\boldsymbol{\chi}^i} \le 1 \quad \forall i = 0, ..., N. \tag{4.56}$$

By standard algebraic calculations, we get

$$\begin{aligned} &\frac{1}{2\tau}\int_\Omega \frac{(P^i)^2}{1+\boldsymbol{\chi}^i} - \frac{1}{2\tau}\int_\Omega \frac{(P^{i-1})^2}{1+\boldsymbol{\chi}^{i-1}} + \frac{1}{2\tau}\int_\Omega \frac{(P^i - P^{i-1})^2}{1+\boldsymbol{\chi}^i} + \int_\Omega \left|\nabla P^i\right|^2 + \int_\Gamma (P^i)^2 \\ &= \frac{1}{\tau}\int_\Omega P^iP^{i-1}\frac{\boldsymbol{\chi}^i - \boldsymbol{\chi}^{i-1}}{(1+\boldsymbol{\chi}^i)(1+\boldsymbol{\chi}^{i-1})} - \frac{1}{2\tau}\int_\Omega (P^{i-1})^2\frac{\boldsymbol{\chi}^i - \boldsymbol{\chi}^{i-1}}{(1+\boldsymbol{\chi}^i)(1+\boldsymbol{\chi}^{i-1})}. \end{aligned} \tag{4.57}$$

Next, we observe that we can find a positive constant C_P such that

$$C_P\left\|P^i\right\|^2_V \le \int_\Omega \left|\nabla P^i\right|^2 + \int_\Gamma (P^i)^2. \tag{4.58}$$

Hence, we multiply (4.57) by τ and get

$$\begin{aligned} &\frac{1}{2}\int_\Omega \frac{(P^i)^2}{1+\boldsymbol{\chi}^i} - \frac{1}{2}\int_\Omega \frac{(P^{i-1})^2}{1+\boldsymbol{\chi}^{i-1}} + \frac{\tau^2}{2}\int_\Omega \left(\frac{P^i - P^{i-1}}{\tau}\right)^2 \frac{1}{1+\boldsymbol{\chi}^i} + C_P\tau\left\|P^i\right\|^2_V \\ &\le \int_\Omega P^iP^{i-1}\frac{\boldsymbol{\chi}^i - \boldsymbol{\chi}^{i-1}}{(1+\boldsymbol{\chi}^i)(1+\boldsymbol{\chi}^{i-1})} - \frac{1}{2}\int_\Omega (P^{i-1})^2\frac{\boldsymbol{\chi}^i - \boldsymbol{\chi}^{i-1}}{(1+\boldsymbol{\chi}^i)(1+\boldsymbol{\chi}^{i-1})}. \end{aligned} \tag{4.59}$$

To handle the first integral on the right-hand side of (4.59) we exploit (4.56), the extended Hölder inequality and Young's inequality to obtain

$$\int_\Omega P^iP^{i-1}\frac{(\boldsymbol{\chi}^i - \boldsymbol{\chi}^{i-1})}{(1+\boldsymbol{\chi}^i)(1+\boldsymbol{\chi}^{i-1})} \le \frac{C_P\tau}{4}\left\|P^i\right\|^2_V + \frac{\tau}{C_P}\left\|\frac{\boldsymbol{\chi}^i - \boldsymbol{\chi}^{i-1}}{\tau}\right\|^2_V \left\|P^{i-1}\right\|^2_H. \tag{4.60}$$

We proceed similarly for the last integral on the right hand side of (4.59) so to get

$$-\frac{1}{2}\int_\Omega \frac{(P^{i-1})^2(\boldsymbol{\chi}^i-\boldsymbol{\chi}^{i-1})}{(1+\boldsymbol{\chi}^i)(1+\boldsymbol{\chi}^{i-1})} \le \frac{C_P\tau}{4}\left\|P^{i-1}\right\|_V^2 + \frac{\tau}{4C_P}\left\|\frac{\boldsymbol{\chi}^i-\boldsymbol{\chi}^{i-1}}{\tau}\right\|_V^2 \left\|P^{i-1}\right\|_H^2. \tag{4.61}$$

Then, combining (4.59)-(4.61) and summing up for $i = 1, ...m$ with $m \le N$, we obtain (see (3.11))

$$\begin{aligned}&\frac{C_\chi}{2}\left\|P^m\right\|_H^2 + \frac{C_\chi}{2}\sum_{i=1}^m \tau^2\left\|\frac{P^i-P^{i-1}}{\tau}\right\|_H^2 + \frac{C_P}{2}\sum_{i=1}^m \tau\left\|P^i\right\|_V^2\\ &\le \frac{1}{2}\left\|p_{0\tau}\right\|_H^2 + \frac{5}{4C_P}\sum_{i=1}^m \tau\left\|\frac{\boldsymbol{\chi}^i-\boldsymbol{\chi}^{i-1}}{\tau}\right\|_V^2\left\|P^{i-1}\right\|_H^2.\end{aligned} \tag{4.62}$$

Hence, we can apply the discrete Gronwall lemma [14, Prop. 2.2.1] and, due to (3.6), (4.36), deduce that

$$\|\bar{p}_\tau\|_{L^\infty(0,T,H)\cap L^2(0,T,V)} \le C. \tag{4.63}$$

Eighth a priori estimate. We test (4.55) by $(P^i - P^{i-1})$. By exploiting once more (4.12), Hölder's and Young's inequalities and similarly proceeding as for (4.49), we write

$$\begin{aligned}&\frac{1}{\tau}\int_\Omega \frac{(P^i-P^{i-1})^2}{1+\boldsymbol{\chi}^i} + \frac{1}{2}\left\|\nabla P^i\right\|_H^2 - \frac{1}{2}\left\|\nabla P^{i-1}\right\|_H^2 + \frac{1}{2}\left\|P^i\right\|_{L^2(\Gamma)}^2\\ &-\frac{1}{2}\left\|P^{i-1}\right\|_{L^2(\Gamma)}^2 \le \frac{1}{\tau}\int_\Omega P^{i-1}(P^i-P^{i-1})\frac{\boldsymbol{\chi}^i-\boldsymbol{\chi}^{i-1}}{(1+\boldsymbol{\chi}^i)(1+\boldsymbol{\chi}^{i-1})}.\end{aligned} \tag{4.64}$$

The integral on the right hand side of (4.64) can be estimated as follows (see (4.56))

$$\begin{aligned}&\frac{1}{\tau}\int_\Omega P^{i-1}(P^i-P^{i-1})\frac{\boldsymbol{\chi}^i-\boldsymbol{\chi}^{i-1}}{(1+\boldsymbol{\chi}^i)(1+\boldsymbol{\chi}^{i-1})}\\ &\le \frac{C_\chi\tau}{2}\left\|\frac{P^i-P^{i-1}}{\tau}\right\|_H^2 + \frac{\tau}{2C_\chi}\left\|P^{i-1}\right\|_V^2\left\|\frac{\boldsymbol{\chi}^i-\boldsymbol{\chi}^{i-1}}{\tau}\right\|_V^2.\end{aligned} \tag{4.65}$$

By combining (4.64) and (4.65), summing up for $i = 1, ..., m$ and exploiting (3.11) along with (4.58), we get

$$\begin{aligned}&\frac{C_\chi}{2}\sum_{i=1}^m \tau\left\|\frac{P^i-P^{i-1}}{\tau}\right\|_H^2 + \frac{C_P}{2}\left\|P^m\right\|_V^2 \le \frac{1}{2}\left\|\nabla p_{0\tau}\right\|_H^2 + \frac{1}{2}\left\|p_{0\tau}\right\|_{L^2(\Gamma)}^2\\ &+\frac{1}{2C_\chi}\sum_{i=1}^m \tau\left\|\frac{\boldsymbol{\chi}^i-\boldsymbol{\chi}^{i-1}}{\tau}\right\|_V^2\left\|P^{i-1}\right\|_V^2.\end{aligned} \tag{4.66}$$

By suitably applying the discrete Gronwall lemma [14, Prop. 2.2.1] it is not difficult to recover the following estimate (see (3.6))

$$\|p_\tau\|_{H^1(0,T,H)} + \|\bar{p}_\tau\|_{L^\infty(0,T,V)} \le C. \tag{4.67}$$

Ninth a priori estimate. Now, we want to achieve the following estimate

$$\|u_\tau\|_{H^1(0,T,H)} \le C. \tag{4.68}$$

To this aim, it suffices to prove that $\|\bar{u}_\tau\|_{L^2(0,T,H)}^2 \le C$ and $\|\partial_t u_\tau\|_{L^2(0,T,H)}^2 \le C$. Thus, in order to check the first estimate, we exploit (2.37), (4.63) and have

$$\|\bar{u}_\tau\|_{L^2(0,T,H)}^2 = \left\|\frac{\bar{p}_\tau}{1+\bar{\chi}_\tau}\right\|_{L^2(0,T,H)}^2 \le \|\bar{p}_\tau\|_{L^2(0,T,H)}^2 \le C. \tag{4.69}$$

Now, let us deal with the second estimate. By virtue of (3.18), (4.56), (4.36) and (4.67), we can write

$$\|\partial_t u_\tau\|_{L^2(0,T,H)}^2 \le 2\left(\|\partial_t p_\tau\|_{L^2(0,T,H)}^2 + \|\bar{p}_\tau\|_{L^\infty(0,T,V)}^2\|\partial_t \chi_\tau\|_{L^2(0,T,V)}^2\right) \le C. \tag{4.70}$$

Thus, combining (4.69)-(4.70) we are able to deduce (4.68). In particular, since $\|\partial_t u_\tau\|_{L^2(0,T,H)} \le C$, a comparison in (4.5) allows us to infer that $\|\mathcal{B}\bar{p}_\tau\|_{L^2(0,T,H)} \le C$ and standard elliptic regularity results yield

$$\|\bar{p}_\tau\|_{L^2(0,T,H^2(\Omega))} \le C. \tag{4.71}$$

In the end, the following estimate

$$\|\bar{u}_\tau\|_{L^\infty(0,T,V)} \le C \tag{4.72}$$

is a consequence of (4.36) and (4.67), since (see (4.6))

$$\begin{aligned} \|\bar{u}_\tau\|^2_{L^\infty(0,T,V)} &= \sup_{(0,T)} \left(\left\| \frac{\bar{p}_\tau}{1+\bar{\chi}_\tau} \right\|_H^2 + \left\| \frac{\nabla \bar{p}_\tau}{1+\bar{\chi}_\tau} - \frac{\bar{p}_\tau \nabla \bar{\chi}_\tau}{(1+\bar{\chi}_\tau)^2} \right\|_H^2 \right) \\ &\le C_{10} \|\bar{p}_\tau\|^2_{L^\infty(0,T,V)} \left(1 + \|\bar{\chi}_\tau\|^2_{L^\infty(0,T,W)}\right) \le C. \end{aligned} \tag{4.73}$$

5. Convergence results

In this section we aim to deduce some convergence results that allow us to pass to the limit as τ tends to 0 in (4.1)-(4.6) and (4.7), (4.10)-(4.11) so to conclude the proof of Theorem 2.3. Since we will obtain a great deal of convergences, we prefer to retrieve them step by step instead of presenting all the results in just one proposition. At first, we can combine the previous estimates (4.31), (4.32), (4.36), (4.39), (4.47), (4.48), (4.49)-(4.54), (4.63), (4.67), (4.68), (4.71), (4.72) so to obtain, on account of (3.1)-(3.2),

$$\|\bar{\chi}_\tau\|_{L^\infty(0,T,W)} + \|\chi_\tau\|_{H^1(0,T,V)} \le c, \tag{5.1}$$
$$\|\bar{e}_\tau\|_{L^\infty(0,T,H)\cap L^2(0,T,V)} + \|e_\tau\|_{W^{1,1}(0,T,V')\cap L^2(0,T,V)} \le c \tag{5.2}$$
$$\left\|\bar{\theta}_\tau\right\|_{L^\infty(0,T,H)\cap L^2(0,T,V)} \le c \tag{5.3}$$
$$\|\bar{u}_\tau\|_{L^\infty(0,T,V)} + \|u_\tau\|_{H^1(0,T,H)} \le c \tag{5.4}$$
$$\|\bar{p}_\tau\|_{L^\infty(0,T,V)\cap L^2(0,T,H^2(\Omega))} + \|p_\tau\|_{H^1(0,T,H)} \le c \tag{5.5}$$
$$\|\log \bar{p}_\tau\|_{L^\infty(0,T,L^1(\Omega))\cap L^2(0,T,V)} \le c \tag{5.6}$$

for c not depending on $\tau \in (0, \hat{\tau})$, for a suitable $\hat{\tau} > 0$.

Now, it remains to pass to the limit in (4.1)-(4.6) and (4.7), (4.10)-(4.11) as $\tau \searrow 0$. An easy computation yields

$$\|\chi_\tau\|_{L^\infty(0,T,W)} \le \|\chi_0\|_W + \|\bar{\chi}_\tau\|_{L^\infty(0,T,W)} \le c, \tag{5.7}$$

and analogous estimates hold for $\|e_\tau\|_{L^\infty(0,T,H)}$, $\|p_\tau\|_{L^\infty(0,T,V)}$ and $\|u_\tau\|_{L^\infty(0,T,V)}$. By virtue of (5.7), well-known weak and weak star compactness results apply to (5.1)-(5.2), (5.4)-(5.5) and ensure the following weak and weak star convergences to hold, possibly for a subsequence of τ,

$$\chi_\tau \overset{*}{\rightharpoonup} \chi \quad \text{in } H^1(0,T,V) \cap L^\infty(0,T,W), \tag{5.8}$$
$$e_\tau \overset{*}{\rightharpoonup} e \quad \text{in } L^\infty(0,T,H) \cap L^2(0,T,V), \tag{5.9}$$
$$u_\tau \overset{*}{\rightharpoonup} u \quad \text{in } H^1(0,T,H) \cap L^\infty(0,T,V), \tag{5.10}$$
$$p_\tau \overset{*}{\rightharpoonup} p \quad \text{in } H^1(0,T,H) \cap L^\infty(0,T,V). \tag{5.11}$$

Let us stress that, even if we do not specify it, the convergence results have to be intended to hold up to the extraction of a suitable subsequence of τ, still denoted by τ for the sake of convenience. Then, owing to strong compactness theorems (see e.g. [24, Cor. 4, p. 85]), by (4.54), (5.8)-(5.11), we get

$$\chi_\tau \to \chi \quad \text{in } C^0([0,T], H^{2-\varepsilon}(\Omega)), \tag{5.12}$$
$$e_\tau \to e \quad \text{in } L^2(0,T,H) \tag{5.13}$$
$$u_\tau \to u \quad \text{and} \quad p_\tau \to p \quad \text{in } C^0([0,T], H^{1-\varepsilon}(\Omega)), \quad \text{if } \varepsilon > 0. \tag{5.14}$$

Moreover, the following relation is fulfilled (cf. (3.1)-(3.2))

$$\|\chi_\tau - \bar{\chi}_\tau\|^2_{L^\infty(0,T,V)} \le \max_{1\le i\le N} \tau^2 \left\| \frac{\chi^i - \chi^{i-1}}{\tau} \right\|^2_H \le \tau \|\partial_t \chi_\tau\|^2_{L^2(0,T,H)} \le \tau c, \tag{5.15}$$

and analogous estimates holds for $\|p_\tau - \bar{p}_\tau\|^2_{L^\infty(0,T,H)}$ and $\|u_\tau - \bar{u}_\tau\|^2_{L^\infty(0,T,H)}$. While for the difference between e_τ and $\bar{e}_\tau$ we have

$$\|e_\tau - \bar{e}_\tau\|_{L^1(0,T,V')} \le \tau \|\partial_t e_\tau\|_{L^1(0,T,V')} \le \tau c. \tag{5.16}$$

Finally, with the help of (5.1)-(5.6), (5.12)-(5.14) and (5.15)-(5.16), we are allowed to infer that

$$\bar{\chi}_\tau \to \chi \quad \text{in } L^\infty(0,T,V), \quad \bar{\chi}_\tau \overset{*}{\rightharpoonup} \chi \quad \text{in } L^\infty(0,T,W), \tag{5.17}$$

$$\bar{e}_\tau \to e \quad \text{in } L^1(0,T,V'), \quad \bar{e}_\tau \overset{*}{\rightharpoonup} e \quad \text{in } L^\infty(0,T,H) \cap L^2(0,T,V), \tag{5.18}$$

$$\bar{\theta}_\tau \overset{*}{\rightharpoonup} \theta \quad \text{in } L^\infty(0,T,H) \cap L^2(0,T,V), \tag{5.19}$$

$$\bar{u}_\tau \to u \quad \text{in } L^\infty(0,T,H), \quad \bar{u}_\tau \overset{*}{\rightharpoonup} u \quad \text{in } L^\infty(0,T,V), \tag{5.20}$$

$$\bar{p}_\tau \to p \quad \text{in } L^\infty(0,T,H), \quad \bar{p}_\tau \overset{*}{\rightharpoonup} p \quad \text{in } L^\infty(0,T,V) \cap L^2(0,T,H^2(\Omega)), \tag{5.21}$$

$$\log \bar{p}_\tau \rightharpoonup y \quad \text{in } L^2(0,T,V), \tag{5.22}$$

where the last limit y will be identified in the sequel.

Now, we want to improve the strong convergence for $\bar{e}_\tau$ in (5.18). To this aim, we first note that

$$\|\bar{e}_\tau - e\|^p_{L^p(0,T,V')} \le \|\bar{e}_\tau - e\|^{p-1}_{L^\infty(0,T,V')} \|\bar{e}_\tau - e\|_{L^1(0,T,V')}, \tag{5.23}$$

where, by virtue of (5.18), $\|\bar{e}_\tau - e\|^{p-1}_{L^\infty(0,T,V')} \le c$ and $\|\bar{e}_\tau - e\|_{L^1(0,T,V')} \to 0$ for all $1 \le p < +\infty$. Thus, we have $\bar{e}_\tau \to e \quad$ in $L^p(0,T,V')$. In addition, we can perform the following estimate

$$\|\bar{e}_\tau - e\|^2_{L^2(0,T,H)} \le \|\bar{e}_\tau - e\|_{L^2(0,T,V)} \|\bar{e}_\tau - e\|_{L^2(0,T,V')} \tag{5.24}$$

and conclude that

$$\bar{e}_\tau \to e \quad \text{in } L^2(0,T,H). \tag{5.25}$$

Finally, since the relation between $\bar{\theta}_\tau$ and $\bar{e}_\tau$ is bi-lipschitz continuous (see (2.42)), from (5.25) and (5.17) we can deduce that $\bar{\theta}_\tau$ is a Cauchy sequence in $L^2(0,T,H)$ which is a complete space. Therefore, recalling the convergence $\bar{\theta}_\tau \overset{*}{\rightharpoonup} \theta$ in $L^\infty(0,T,H) \cap L^2(0,T,V)$, by uniqueness of the limit we conclude that

$$\bar{\theta}_\tau \to \theta \quad \text{in } L^2(0,T,H). \tag{5.26}$$

Now, by virtue of the above convergences (5.25), (5.26), (5.17) and owing to the properties of ψ (see (2.42)-(2.43)), it is easy to recover (2.25) from (4.2), i.e. $e = \psi(\theta, \chi)$.

Next, we deal with the logarithmic term in (4.3). Thanks to the strong convergence in (5.21), there exists a subsequence still denoted by $\bar{p}_\tau$ such that

$$\bar{p}_\tau \to p \quad \text{a.e. in } Q, \tag{5.27}$$

and consequently such that

$$\log \bar{p}_\tau \to \log p \quad \text{a.e. in } Q. \tag{5.28}$$

In principle, the a.e. limit of $\log \bar{p}_\tau$ could be $-\infty$ in a subset of positive measure (in which $p = 0$): but the property

$$\int_Q |\log \bar{p}_\tau|^2 \le c \quad \forall \tau$$

and the Fatou lemma imply that

$$\int_Q |\log p|^2 \le \liminf_{\tau \searrow 0} \int_Q |\log \bar{p}_\tau|^2 \le c,$$

whence $\log p$ is well defined. Actually, we are now about to show that the weak limit y of the sequence $\log \bar{p}_\tau$ coincides with the a.e. limit, i.e. with $\log p$. By virtue of (5.28), we can invoke the Severini-Egorov theorem and deduce that for all $\varepsilon > 0$ there exists a set $Q_\varepsilon \subset Q$ such that $\text{meas}(Q_\varepsilon) < \varepsilon$ and

$$\log \bar{p}_\tau \to \log p \quad \text{uniformly in } Q \setminus Q_\varepsilon. \tag{5.29}$$

In addition, since (5.6) holds, a standard interpolation calculus and the continuous embedding $V \subset L^6(\Omega)$ yield

$$\begin{aligned}\|\log \bar{p}_\tau\|_{L^{8/3}(Q)}^{8/3} &\le \int_0^T \left\| |\log \bar{p}_\tau|^{\frac{2}{3}} \right\|_{L^{3/2}(\Omega)} \left\| |\log \bar{p}_\tau|^2 \right\|_{L^3(\Omega)} \\ &\le \|\log \bar{p}_\tau\|_{L^\infty(0,T,L^1(\Omega))}^{2/3} \|\log \bar{p}_\tau\|_{L^2(0,T,L^6(\Omega))} \\ &\le \|\log \bar{p}_\tau\|_{L^\infty(0,T,L^1(\Omega))}^{2/3} \|\log \bar{p}_\tau\|_{L^2(0,T,V)} \le c,\end{aligned}$$

whence

$$\|\log \bar{p}_\tau\|_{L^{8/3}(Q)} \le c. \tag{5.30}$$

By virtue of (5.29)-(5.30) and of the Hölder inequality, if $1 \le q < 8/3$ we can write

$$\int_Q |\log \bar{p}_\tau - \log p|^q \le \left(\int_{Q_\varepsilon} |\log \bar{p}_\tau - \log p|^{8/3} \right)^{\frac{3q}{8}} \varepsilon^{1-\frac{3q}{8}} + \int_{Q \setminus Q_\varepsilon} |\log \bar{p}_\tau - \log p|^q,$$

and then

$$\lim_{\tau \searrow 0} \int_Q |\log \bar{p}_\tau - \log p|^q \le \sup_\tau \left(\int_Q |\log \bar{p}_\tau - \log p|^{8/3} \right)^{\frac{3q}{8}} \varepsilon^{1-\frac{3q}{8}} \le C\varepsilon^{1-\frac{3q}{8}}.$$

Taking the limit as $\varepsilon \searrow 0$ we obtain $\log \bar{p}_\tau \to \log p \quad \text{in } L^q(Q) \quad \forall 1 \le q < \frac{8}{3}$, and in particular

$$\log \bar{p}_\tau \to \log p \quad \text{in } L^2(Q), \tag{5.31}$$

as $\tau \searrow 0$. Then, owing to Proposition 7.1, the same convergence easily holds (see (3.2) and (3.4)) for $\mathcal{T}_\tau \log(\bar{p}_\tau)$. Besides, we can identify the weak limit y (see (5.22)): the convergence in (5.31) definitely yields $y = \log p$.

Now, by the above convergences, we are in the position of taking the limit as $\tau \searrow 0$ in (4.1)-(4.6) and (4.7), (4.10)-(4.11). At first, we observe that (see (2.35) and (3.5))

$$p_\tau(0) = p_{0\tau} \to p_0 \quad \text{in } H. \tag{5.32}$$

Thanks to (4.7), (4.10)-(4.11), (5.32), (5.8) and (5.10), the limit functions χ, e, u satisfy the initial conditions (1.41), (2.31)-(2.32). The rest of the proof will proceed in five steps. As first, we will pass to the limit in (4.3); secondly we will prove that the following strong convergence holds

$$\partial_t \chi_\tau \to \chi_t \quad \text{in } L^2(0,T,V). \tag{5.33}$$

Then, by virtue of (5.33) we will discuss the passage to the limit in (4.1). Finally we will consider (4.5) and we will easily recover (2.28) by virtue of the above convergences.

In order to pass to the limit in (4.3), we first observe that (5.26) combined with (2.39) yields (see Proposition 7.1)

$$h(\mathcal{T}_\tau \bar{\theta}_\tau) \to h(\theta) \quad \text{in } L^2(Q). \tag{5.34}$$

Thus, by virtue of (5.8), (5.17), (5.31) and (5.34), in order to conclude the passage to the limit as $\tau \searrow 0$ in (4.3), it suffices to control the sequence $\bar{\xi}_\tau$. In particular we need to verify that $\bar{\xi}_\tau$ converges, in a suitable sense, to some selection $\xi \in \partial_{V,V'} J(\chi)$. To this aim, we observe that, by a comparison in (4.3), (2.39), (5.1) and (5.6) imply

$$\|\bar{\xi}_\tau\|_{L^2(0,T,V')} \le c, \tag{5.35}$$

and consequently we have

$$\bar{\xi}_\tau \rightharpoonup \xi \quad \text{in } L^2(0,T,V'). \tag{5.36}$$

Hence, by (5.17) and (5.36) we can deduce

$$\int_0^T \langle \bar{\xi}_\tau, \bar{\chi}_\tau \rangle \to \int_0^T \langle \xi, \chi \rangle, \tag{5.37}$$

as $\tau \searrow 0$, which enables us to apply the result presented in [8, Prop. 2.5, p. 27] for $X = L^2(0,T,V)$ and deduce

$$\xi \in \partial_{V,V'} J(\chi) \quad \text{a.e. in } (0,T). \tag{5.38}$$

Indeed, it is known that a maximal monotone operator from V to V' induces an analogous operator from $L^2(0,T,V)$ to $L^2(0,T,V')$ which is defined by the a.e. relation in $(0,T)$. Moreover, in our framework we can refer to [8, Ex. 2.3.3, p. 25] and deduce that the induced operator from $L^2(0,T,V)$ to $L^2(0,T,V')$ is maximal monotone as well. Finally, by the above arguments we can pass to the limit in (4.3) and get (2.26) solved by χ, θ, p in V' and a.e. in (0,T). Now, we aim to prove (5.33). We first note that, since (5.8) holds we can infer that

$$\partial_t \chi_\tau \rightharpoonup \chi_t \quad \text{in } L^2(0,T,V). \tag{5.39}$$

As a consequence, (5.33) can be obtained just by verifying that

$$\limsup_{\tau \searrow 0} \|\partial_t \chi_\tau\|^2_{L^2(0,T,V)} \leq \|\chi_t\|^2_{L^2(0,T,V)}\,, \tag{5.40}$$

since the strong convergence of the norms combined with the weak convergence imply the required strong convergence (5.33). To obtain (5.40) we test (4.3) by $\partial_t \chi_\tau$, integrate over $(0,T)$, and take the lim sup as $\tau \searrow 0$. We have

$$\begin{aligned}\limsup_{\tau \searrow 0} \int_0^T \|\partial_t \chi_\tau\|^2_H + \nu \|\nabla \partial_t \chi_\tau\|^2_H = \limsup_{\tau \searrow 0} \Bigg(&- \int_Q \nabla \bar{\chi}_\tau \nabla \partial_t \chi_\tau - \int_0^T \langle \bar{\xi}_\tau, \partial_t \chi_\tau \rangle \\ &+ \int_Q h(\mathcal{T}_\tau \bar{\theta}_\tau) \partial_t \chi_\tau - \int_Q \mathcal{T}_\tau (\log \bar{p}_\tau) \partial_t \chi_\tau \Bigg).\end{aligned} \tag{5.41}$$

We first note that, since (5.8), (5.17), (5.34) and (5.31) hold, we can infer that

$$\begin{aligned}&\lim_{\tau \searrow 0} \left(- \int_Q \nabla \bar{\chi}_\tau \nabla \partial_t \chi_\tau + \int_Q h(\mathcal{T}_\tau \bar{\theta}_\tau) \partial_t \chi_\tau - \int_Q \mathcal{T}_\tau (\log \bar{p}_\tau) \partial_t \chi_\tau \right) \\ &= - \int_Q \nabla \chi \nabla \chi_t + \int_Q h(\theta) \chi_t - \int_Q (\log p) \chi_t.\end{aligned} \tag{5.42}$$

Next, we have to treat the term $-\int_0^T \langle \bar{\xi}_\tau, \partial_t \chi_\tau \rangle$. To this aim, we observe that by definition of subdifferential and owing to (3.1)-(3.2), we can write

$$\int_0^T \langle \bar{\xi}_\tau, \partial_t \chi_\tau \rangle = \sum_{i=1}^N \langle \Xi^i, \boldsymbol{\chi}^i - \boldsymbol{\chi}^{i-1} \rangle \geq \sum_{i=1}^N J(\boldsymbol{\chi}^i) - J(\boldsymbol{\chi}^{i-1}) = J(\chi_\tau(T)) - J(\chi_0) \tag{5.43}$$

for any $\tau \geq 0$. Hence, by the lower semicontinuity in V of the function J and due to (5.12), we claim that

$$\limsup_{\tau \searrow 0} - \int_0^T \langle \bar{\xi}_\tau, \partial_t \chi_\tau \rangle \leq -J(\chi(T)) + J(\chi_0). \tag{5.44}$$

Hence, by combining (5.42) and (5.44) we get

$$\begin{aligned}&\limsup_{\tau \searrow 0} \left(- \int_Q \nabla \bar{\chi}_\tau \nabla \partial_t \chi_\tau - \int_0^T \langle \bar{\xi}_\tau, \partial_t \chi_\tau \rangle + \int_Q h(\mathcal{T}_\tau \bar{\theta}_\tau) \partial_t \chi_\tau - \int_Q \mathcal{T}_\tau (\log \bar{p}_\tau) \partial_t \chi_\tau \right) \\ &\leq - \int_Q \nabla \chi \nabla \chi_t + \int_Q h(\theta) \chi_t - \int_Q (\log p) \chi_t - J(\chi(T)) + J(\chi_0),\end{aligned} \tag{5.45}$$

and the right hand side of (5.45) is equal to

$$\int_0^T \|\chi_t\|^2_H + \nu \|\nabla \chi_t\|^2_H\,, \tag{5.46}$$

as one can easily verify by testing (2.26) by χ_t and then integrating in time. Thus (5.33) is proved.

Remark 5.1. *The last result follows once proved that*

$$-J(\chi(T)) + J(\chi_0) = - \int_0^T \langle \xi, \chi_t \rangle. \tag{5.47}$$

This can be obtained by extending the statement in [8, Lemma 3.3, p. 73] *to the case of abstract subdifferential operators defined in the duality pairing between V' and V.*

Now, we discuss how to perform the passage to the limit in (4.1). By virtue of (5.19) we have

$$\mathcal{A} \bar{\theta}_\tau \rightharpoonup \mathcal{A} \theta \quad \text{in } L^2(0,T,V'). \tag{5.48}$$

In addition, owing to (5.34) and (5.33) we may infer that

$$\begin{aligned} &h(\mathcal{T}_\tau\bar{\theta}_\tau)\partial_t\chi_\tau \to h(\theta)\chi_t \quad \text{in } L^1(0,T,L^{3/2}(\Omega)),\\ &\partial_t\chi_\tau^2 \to \chi_t^2 \quad \text{in } L^1(0,T,H). \end{aligned} \tag{5.49}$$

Thus, by a comparison in (4.1) we can deduce that

$$\partial_t e_\tau \rightharpoonup \eta \quad \text{in } L^1(0,T,V'), \tag{5.50}$$

where $\eta = -\mathcal{A}\theta - h(\theta)\chi_t + \chi_t^2$. In order to show that $\eta = e_t$ we argue as follows. We consider the time convolution product $1 * (\partial_t e_\tau)$ which satisfies

$$1 * (\partial_t e_\tau) = e_\tau - e_0. \tag{5.51}$$

Then, we observe that the following convergences hold thanks to (5.50)

$$1 * (\partial_t e_\tau) \rightharpoonup 1 * \eta \quad \text{in } W^{1,1}(0,T,V'),$$

while

$$e_\tau - e_0 \overset{*}{\rightharpoonup} e - e_0 \quad \text{in } L^\infty(0,T,H).$$

The uniqueness of the limit of (5.51) entails

$$e = e_0 + 1 * \eta. \tag{5.52}$$

Hence, e must be derivable and, by deriving (5.52), we get $e_t = \eta$. Thus, we can pass to the limit in (4.1) getting (2.24).

Finally, we aim to take the limit in (4.5)-(4.6). On account of (5.21) it is easily verified that

$$\mathcal{B}\bar{p}_\tau \overset{*}{\rightharpoonup} \mathcal{B}p \quad \text{in } L^\infty(0,T,V') \cap L^2(0,T,H). \tag{5.53}$$

On the other hand, thanks to (5.10), we have

$$\partial_t u_\tau \rightharpoonup u_t \quad \text{in } L^2(0,T,H). \tag{5.54}$$

As a consequence of (5.53) and (5.54) we can pass to the limit in (4.5) and get (2.28). Finally, we equivalently rewrite (4.6) as follows

$$\bar{u}_\tau = \frac{1}{1+\bar{\chi}_\tau}\,(\bar{p}_\tau - p) + p\left(\frac{1}{1+\bar{\chi}_\tau}\right). \tag{5.55}$$

Let us note that (5.17), (5.21) and the fact that $\bar{\chi}_\tau \in L^\infty(Q)$ allow us to take the limit as $\tau \searrow 0$ in (5.55) and eventually get (2.29). Then Theorem 2.3 is completely proved.

6. Regularity results

This section is devoted to the proof of Theorems 2.4, 2.5 and 2.6. The proof of the improved regularities is based on formal estimates performed on the solutions of the complete dissipative model (2.24)-(2.29). Actually, the following estimates can be made rigorous and, in particular, the proof of Theorem 2.5 can be directly reproduced on the discrete scheme.

As first, we prove Theorem 2.4 that states a further regularity for the inverse of the pressure p^{-1}. We first achieve an improved regularity for the variable u^{-1} by means of a formal estimate, then we will deduce the required result for p^{-1}.

Before proceeding, for $n \le 3$, we recall the Sobolev embedding $H^1(\Omega) \hookrightarrow L^6(\Omega)$ and the Gagliardo-Niremberg inequality (cf. [21]), yielding, for $n = 3$,

$$\|v\|^2_{L^3(\Omega)} \le C_{\mathrm{GN}}\,\|v\|_H\,\|\nabla v\|_H + C'_{\mathrm{GN}}\,\|v\|^2_H\,. \tag{6.1}$$

Now, we consider (2.28) rewritten in the terms of the variables u and χ as

$$u_t + \mathcal{B}(u(1+\chi)) = 0. \tag{6.2}$$

We formally test (6.2) by $-u^{-3}$ and integrate over $(0,t)$. For a rigorous estimate, we could proceed as in the First a priori estimate of Chapter 4. In particular, we could truncate the function $-u^{-3}$ at level ε and then let ε tend to zero. Let us note that, by virtue of (2.32), (2.34) and (2.52) we get $u_0^{-1} = (1+\chi_0)p_0^{-1} \in H$. We first have

$$-\int_0^t \int_\Omega u_t u^{-3} = \frac{1}{2}\int_0^t \int_\Omega \frac{\partial}{\partial t}(u^{-2}) = \frac{1}{2}\left\|u^{-1}(t)\right\|_H^2 - \frac{1}{2}\left\|u_0^{-1}\right\|_H^2. \tag{6.3}$$

Then, by definition of $\mathcal{B}$, we write

$$\begin{aligned} &-\int_0^t \langle \mathcal{B}(u(1+\chi)), u^{-3}\rangle \\ &= 3\int_0^t \int_\Omega (1+\chi)\left|\nabla u\right|^2 u^{-4} - \int_0^t \int_\Gamma u^{-2}(1+\chi) + 3\int_0^t \int_\Omega u^{-3}\nabla u \nabla \chi. \end{aligned} \tag{6.4}$$

The third integral on the right hand side of (6.4) is estimated as follows (see (6.1))

$$\begin{aligned} &3\int_0^t \int_\Omega \left|u^{-3}\nabla u\nabla\chi\right| \le 3\int_0^t \|\nabla\chi\|_{L^6(\Omega)} \left\|\nabla(u^{-1})\right\|_H \left\|u^{-1}\right\|_{L^3(\Omega)} \\ &\le \frac{3}{4}\left\|\nabla(u^{-1})\right\|_{L^2(0,t,H)}^2 + 3C_{\mathrm{GN}}\int_0^t \|\nabla\chi\|_{L^6(\Omega)}^2 \left\|u^{-1}\right\|_H \left\|\nabla(u^{-1})\right\|_H \\ &+ 3C'_{\mathrm{GN}}\int_0^t \|\nabla\chi\|_{L^6(\Omega)}^2 \left\|u^{-1}\right\|_H^2. \end{aligned} \tag{6.5}$$

Now, since $\nabla\chi \in L^\infty(0,T,V)$ (cf. (2.47)), with the help of Young's inequality, we can eventually write

$$3\int_0^t \int_\Omega \left|u^{-3}\nabla u\nabla\chi\right| \le C_{11} + \frac{3}{2}\left\|\nabla(u^{-1})\right\|_{L^2(0,t,H)}^2 + C_{12}\int_0^t \left\|u^{-1}\right\|_H^2. \tag{6.6}$$

As the trace operator $\gamma : V \to L^2(\Gamma)$ is compact, we may deduce that, for any $\sigma > 0$, there exists $c_\sigma > 0$ such that

$$\|\gamma(v)\|_{L^2(\Gamma)}^2 \le \sigma\|v\|_V^2 + C_\sigma\|v\|_H^2 \quad \forall v \in V. \tag{6.7}$$

Thus, we can control the boundary integral in (6.4) as follows

$$\left|\int_0^t \int_\Gamma u^{-2}(1+\chi)\right| \le \sigma\left\|\nabla u^{-1}\right\|_{L^2(0,t,H)}^2 + C_\sigma\left\|u^{-1}\right\|_{L^2(0,t,H)}^2. \tag{6.8}$$

Finally we point out that for the first integral on the right hand side of (6.4) the following equality holds

$$3\int_0^t \int_\Omega (1+\chi)\left|\nabla u\right|^2 u^{-4} = 3\int_0^t \int_\Omega (1+\chi)\left|\nabla(u^{-1})\right|^2. \tag{6.9}$$

Combining (6.2)-(6.8) for a sufficiently small σ, we have

$$\left\|u^{-1}(t)\right\|_H^2 + \left\|\nabla(u^{-1})\right\|_{L^2(0,t,H)}^2 \le C_{13}\left(1 + \int_0^t \left\|u^{-1}\right\|_H^2\right). \tag{6.10}$$

We can apply the Gronwall lemma [2, Theorem 2.1] to (6.10) and finally obtain

$$\left\|u^{-1}\right\|_{L^\infty(0,T,H)\cap L^2(0,T,V)} \le c. \tag{6.11}$$

The same estimate can be derived for the inverse of the pressure p^{-1}. Indeed, thanks to (2.47) and to the relation $p^{-1} = u^{-1}(1+\chi)^{-1}$, we can easily deduce that (6.11) implies

$$\left\|p^{-1}\right\|_{L^\infty(0,T,H)\cap L^2(0,T,V)} \le c. \tag{6.12}$$

Let us detail such a procedure. By virtue of the Hölder inequality and of the continuous embedding $V \subset L^4(\Omega)$, we have

$$\begin{aligned} \left\|p^{-1}\right\|_{L^2(0,T,V)}^2 &= \int_0^T \left\|\frac{u^{-1}}{1+\chi}\right\|_H^2 + \int_0^T \left\|\frac{\nabla u^{-1}}{1+\chi} - \frac{u^{-1}\nabla\chi}{(1+\chi)^2}\right\|_H^2 \\ &\le C_{14}\left(\left\|u^{-1}\right\|_{L^2(0,T,V)}^2 + \int_0^T \left\|u^{-1}\right\|_{L^4(\Omega)}^2 \|\nabla\chi\|_{L^4(\Omega)}^2\right) \\ &\le C_{15}\left(\left\|u^{-1}\right\|_{L^2(0,T,V)}^2 + \|\chi\|_{L^\infty(0,T,W)}^2 \left\|u^{-1}\right\|_{L^2(0,T,V)}^2\right) \le c. \end{aligned} \tag{6.13}$$

Analogously, we can easily deduce that $\left\|p^{-1}\right\|^2_{L^\infty(0,T,H)} \leq \left\|u^{-1}\right\|^2_{L^\infty(0,T,H)}$. From (6.13) we can eventually infer that (6.12) holds and Theorem 2.4 is consequently proved.

In order to prove Theorem 2.5 we perform a further a priori estimate, that can be suitably reproduced on the discrete scheme. Let us deal with (2.24) and rewrite it as

$$(1+\chi\theta h''(\theta))\theta_t + \mathcal{A}\theta = -\theta h'(\theta)\chi_t + \chi_t^2. \tag{6.14}$$

Now, we test (6.14) by θ_t, integrate over $(0,t)$ and get

$$\int_0^t\int_\Omega \theta_t^2(1+\chi\theta h''(\theta)) + \int_0^t \langle\mathcal{A}\theta,\theta_t\rangle = -\int_0^t\int_\Omega \theta h'(\theta)\theta_t\chi_t + \int_0^t\int_\Omega \chi_t^2\theta_t. \tag{6.15}$$

Owing to (2.40)-(2.41) we obtain

$$c_s\left\|\theta_t\right\|^2_{L^2(0,t,H)} \leq \int_0^t\int_\Omega \theta_t^2(1+\chi\theta h''(\theta)) \tag{6.16}$$

and

$$\begin{aligned}
&\left|\int_0^t\int_\Omega \theta h'(\theta)\theta_t\chi_t\right| + \left|\int_0^t\int_\Omega \chi_t^2\theta_t\right| \leq c_h\int_0^t\int_\Omega |\chi_t|\,|\theta_t| + \int_0^t\int_\Omega |\chi_t|^2\,|\theta_t| \\
&\leq C_{16}\int_0^t\left(\left\|\chi_t\right\|_H + \left\|\chi_t\right\|_V^2\right)\left\|\theta_t\right\|_H \\
&\leq \frac{c_s}{2}\left\|\theta_t\right\|^2_{L^2(0,t,H)} + C_{17}\int_0^t\left\|\chi_t\right\|_H^2 + C_{18}\int_0^t\left\|\chi_t\right\|_V^2\left\|\chi_t\right\|_V^2,
\end{aligned} \tag{6.17}$$

where we have exploited the Young and Hölder inequalities as well as the continuous embedding $V \subset L^4(\Omega)$. By integrating by parts in time, thanks to (2.33) it follows that

$$\frac{c_s}{2}\left\|\theta_t\right\|^2_{L^2(0,t,H)} + \frac{1}{2}\left\|\nabla\theta(t)\right\|_H^2 \leq C_{19} + C_{17}\int_0^t\left\|\chi_t\right\|_H^2 + C_{18}\int_0^t\left\|\chi_t\right\|_V^2\left\|\chi_t\right\|_V^2, \tag{6.18}$$

where for the moment we just know that $\left\|\chi_t\right\|_V^2 \in L^1(0,T)$ (see (2.47)). However, we are going to combine estimate (6.18) with another estimate which will give us more information on $\left\|\chi_t\right\|_V^2$. Indeed, we consider (2.26) and differentiate it with respect to time thus obtaining

$$\chi_{tt} + \nu\mathcal{A}\chi_{tt} + \mathcal{A}\chi_t + \xi_t = h'(\theta)\theta_t - \frac{1}{p}p_t. \tag{6.19}$$

Then, we test (6.19) by χ_t. After some integrations by parts in time and owing to (2.39), we can write

$$\begin{aligned}
&\frac{1}{2}\int_\Omega\left(|\chi_t|^2 + \nu|\nabla\chi_t|^2\right)(t) + \int_0^t\int_\Omega |\nabla\chi_t|^2 + \int_0^t\langle\xi_t,\chi_t\rangle \\
&\leq C_{20}\left\|\chi_t(0)\right\|_V^2 + c_h\int_0^t\int_\Omega |\theta_t|\,|\chi_t| + \int_0^t\int_\Omega\left|\frac{1}{p}\right||p_t|\,|\chi_t|.
\end{aligned} \tag{6.20}$$

Let us note that since $\chi_0 \in D(\partial_{V,V'}J)$, there exists $\xi_0 \in \partial_{V,V'}J(\chi_0)$. Thus, we can introduce χ_0' as the initial value of the time derivative of χ by defining it as the solution of the following elliptic equation

$$\chi_0' + \nu\mathcal{A}\chi_0' = -\mathcal{A}\chi_0 - \xi_0 + h(\theta_0) - \log p_0, \tag{6.21}$$

where the right hand side is known in V' thanks to (2.33)-(2.35), (2.39) and (2.52). Then, it easily follows that $\chi_0' \in V$. Next, we observe that monotonicity arguments yield

$$\int_0^t\langle\xi_t,\chi_t\rangle \geq 0. \tag{6.22}$$

By applying Hölder's and Young's inequalities, we can estimate the first integral on the right hand side of (6.20) as follows

$$c_h\int_0^t\int_\Omega |\theta_t|\,|\chi_t| \leq \frac{c_s}{4}\left\|\theta_t\right\|^2_{L^2(0,t,H)} + C_{21}\int_0^t\left\|\chi_t\right\|_H^2. \tag{6.23}$$

Analogously, the last integral on the right hand side of (6.20) can be handled as follows

$$\int_0^t\int_\Omega\left|\frac{1}{p}\right||p_t|\,|\chi_t| \leq \int_0^t\left\|\frac{1}{p}\right\|_{L^4(\Omega)}\left\|p_t\right\|_H\left\|\chi_t\right\|_V, \tag{6.24}$$

where, owing to Theorems 2.3 and 2.4, $(\|1/p\|_{L^4(\Omega)} \|p_t\|_H) \in L^1(0,T)$. Thanks to (6.22)-(6.24), (6.20) yields

$$\begin{aligned}&\frac{1}{2}\int_\Omega \left(|\chi_t|^2 + \nu |\nabla \chi_t|^2\right)(t) + \int_0^t \int_\Omega |\nabla \chi_t|^2 \\ &\le C_{22} + \frac{c_s}{4}\|\theta_t\|^2_{L^2(0,t,H)} + C_{21}\int_0^t \|\chi_t\|_H^2 + \int_0^t \left\|\frac{1}{p}\right\|_{L^4(\Omega)} \|p_t\|_H \|\chi_t\|_V . \end{aligned} \tag{6.25}$$

Finally, by combining (6.18) and (6.25), we obtain

$$\begin{aligned}&\frac{c_s}{4}\|\theta_t\|^2_{L^2(0,t,H)} + \frac{1}{2}\|\nabla\theta(t)\|_H^2 + \frac{1}{2}\int_\Omega \left(|\chi_t|^2 + \nu |\nabla \chi_t|^2\right)(t) + \|\nabla \chi_t\|^2_{L^2(0,t,H)} \\ &\le C_{23} + C_{18}\int_0^t \|\chi_t\|_V^2 \|\chi_t\|_V^2 + C_{24}\int_0^t \|\chi_t\|_H^2 + \int_0^t \left\|\frac{1}{p}\right\|_{L^4(\Omega)} \|p_t\|_H \|\chi_t\|_V . \end{aligned} \tag{6.26}$$

Now, we can apply the Gronwall lemma [2, Theorem 2.1] and owing to Theorem 2.3 (see (2.45) and (2.47)) we get

$$\|\theta\|_{H^1(0,T,H)\cap L^\infty(0,T,V)} + \|\chi\|_{W^{1,\infty}(0,T,V)} \le c, \tag{6.27}$$

so that Theorem 2.5 is completely proved.

Finally, we aim to prove Theorem 2.6, i.e. to establish the positivity of the temperature. To this purpose, we deal with (6.14) and formally test it by $-\theta^{-1}$. After integrating over $(0,t)$, for the first term we get

$$\begin{aligned}-\int_0^t \int_\Omega \theta_t \theta^{-1} &= -\int_0^t \int_\Omega \frac{d}{dt}(\log\theta) \\ &= \int_\Omega (\log\theta)^-(t) - \int_\Omega (\log\theta)^+(t) + \int_\Omega \log\theta_0, \end{aligned} \tag{6.28}$$

where $(\log\theta)^-$ and $(\log\theta)^+$ denote the negative and positive parts of the function $\log\theta$, respectively. Hence, we have

$$\begin{aligned}&\int_\Omega |\log\theta|(t) - \int_0^t\int_\Omega h''(\theta)\theta_t\chi + \int_0^t\int_\Omega |\nabla \log\theta|^2 + \int_0^t\int_\Omega \frac{\chi_t^2}{\theta} \\ &= 2\int_\Omega (\log\theta)^+(t) - \int_\Omega \log\theta_0 + \int_0^t\int_\Omega h'(\theta)\chi_t. \end{aligned} \tag{6.29}$$

Now, we deal with the second integral on the left hand side of (6.29) and, after integrating by parts in time, we can write

$$\begin{aligned}-\int_0^t\int_\Omega h''(\theta)\theta_t\chi &= -\int_0^t\int_\Omega \frac{\partial}{\partial t}(h'(\theta))\chi \\ &= -\int_\Omega h'(\theta(t))\chi(t) + \int_\Omega h'(\theta_0)\chi_0 + \int_0^t\int_\Omega h'(\theta)\chi_t, \end{aligned} \tag{6.30}$$

and then

$$\begin{aligned}&\int_\Omega |\log\theta|(t) + \int_0^t\int_\Omega |\nabla\log\theta|^2 + \int_0^t\int_\Omega \frac{\chi_t^2}{\theta} \\ &= \int_\Omega h'(\theta(t))\chi(t) + 2\int_\Omega (\log\theta)^+(t) - \int_\Omega \log\theta_0 - \int_\Omega h'(\theta_0)\chi_0. \end{aligned} \tag{6.31}$$

Let us observe that well-known properties of the logarithm function and (2.45) yield

$$\begin{aligned}\left\|(\log\theta)^+\right\|_{L^\infty(0,T,L^1(\Omega))} &\le \sup_{0\le t\le T}\int_{\Omega\cap\{\theta\ge 1\}} |\log\theta(t)| \\ &\le \sup_{0\le t\le T}\int_{\Omega\cap\{\theta\ge 1\}} |\theta|^2 \le \|\theta\|^2_{L^\infty(0,T,H)} \le c. \end{aligned} \tag{6.32}$$

Besides, we note that the first integral in the right hand side of (6.31) is bounded thanks to (2.39) and (2.47). By virtue of (2.34), (2.57) and (6.32) we can eventually infer that

$$\|\log\theta(t)\|_{L^1(\Omega)} + \|\nabla\log\theta\|^2_{L^2(0,T,H)} + \left\|\frac{\chi_t}{\sqrt{\theta}}\right\|^2_{L^2(0,T,H)} \leq c. \tag{6.33}$$

As a consequence of (6.32), (6.33) and exploiting the Poincaré-Wirtinger inequality, we can deduce

$$\|\log\theta\|_{L^\infty(0,T,L^1(\Omega))\cap L^2(0,T,V)} + \left\|\frac{\chi_t}{\sqrt{\theta}}\right\|^2_{L^2(0,T,H)} \leq c. \tag{6.34}$$

7. Appendix

In this appendix, we present two auxiliary results among those exploited in our proofs. As first, let us detail and prove a convergence result we have applied in order to pass to the limit in the time discretization scheme.

Proposition 7.1. *Let $\mathcal{T}_\tau$ be the translation operator defined in* (3.4)*. If the sequence $\{v_\tau\}$ satisfies*

$$v_\tau \to v \quad in \quad L^2(-T,T,H), \tag{7.1}$$

as $\tau \searrow 0$, then the following convergence

$$\int_0^T \|\mathcal{T}_\tau v_\tau(t) - v(t)\|^2_H\,dt \xrightarrow[\tau\searrow 0]{} 0 \tag{7.2}$$

holds.

Proof. Here, we give just an outline of the proof. A first step consists in proving that the following convergence

$$\int_0^T \|\mathcal{T}_\tau w(t) - w(t)\|^2_H\,dt \xrightarrow[\tau\searrow 0]{} 0 \tag{7.3}$$

holds for any $w \in C^0([-T,T],H)$[2]. To this aim, let us note that, if $w \in C^0([-T,T],H)$, then (7.3) easily follows by suitably applying the Lebesgue's dominated convergence theorem. Now, since $C^0([-T,T],H)$ is dense in $L^2(-T,T,H)$, if $v \in L^2(-T,T,H)$, there exists an approximating sequence $\{v_n\}_{n\in\mathbb{N}} \subset C^0([-T,T],H)$ such that

$$v_n \to v \quad \text{in} \quad L^2(-T,T,H) \tag{7.4}$$

as $n \to +\infty$. In particular, for any $\varepsilon > 0$, there exists $n_\varepsilon \in \mathbb{N}$ such that the inequality

$$\|v_n - v\|^2_{L^2(-T,T,H)} \leq \varepsilon \tag{7.5}$$

holds for all $n \geq n_\varepsilon$. Moreover, thanks to (3.4), from (7.5) we can easily deduce that

$$\int_0^T \|\mathcal{T}_\tau v_n(t) - \mathcal{T}_\tau v(t)\|^2_H\,dt \leq \|v_n - v\|^2_{L^2(-T,T,H)} \leq \varepsilon \tag{7.6}$$

for all $n \geq n_\varepsilon$ and for all $0 < \tau < T$. Now, we fix $n = n_\varepsilon$ and point out that since $v_n \in C^0([-T,T],H)$ then (7.3) holds for $w = v_n$. In particular, there exists τ_ε such that

$$\int_0^T \|\mathcal{T}_\tau v_n(t) - v_n(t)\|^2_H\,dt \leq \varepsilon \tag{7.7}$$

for all $\tau \leq \tau_\varepsilon$. This allows us to split the difference $(\mathcal{T}_\tau v - v)$ into three terms, all tending to zero in $L^2(0,T,H)$. Namely, we can write

$$\begin{aligned} \mathcal{T}_\tau v - v = {} & \mathcal{T}_\tau v - \mathcal{T}_\tau v_n \\ & + \mathcal{T}_\tau v_n - v_n \\ & + v_n - v. \end{aligned} \tag{7.8}$$

[2]By $C^0([-T,T],H)$ we denote the space of continuous functions from $[-T,T]$ into H equipped with the $L^\infty(-T,T,H)$ norm.

By means of the above arguments, we can infer that the following inequality

$$\int_0^T \|\mathcal{T}_\tau v(t) - v(t)\|_H^2\,dt \le 3\varepsilon \tag{7.9}$$

holds for all $\tau \le \tau_\varepsilon$, whence

$$\int_0^T \|\mathcal{T}_\tau v(t) - v(t)\|_H^2\,dt \xrightarrow[\tau\searrow 0]{} 0. \tag{7.10}$$

Finally, we consider the difference between $\mathcal{T}_\tau v_\tau$ and v. It is convenient to express it as follows

$$\begin{aligned}\mathcal{T}_\tau v_\tau - v &= \mathcal{T}_\tau v_\tau - \mathcal{T}_\tau v\\ &\quad + \mathcal{T}_\tau v - v.\end{aligned} \tag{7.11}$$

Thanks to (7.1) and to the definition of $\mathcal{T}_\tau$, for the first addend on the right hand side we can write

$$\int_0^T \|\mathcal{T}_\tau v_\tau(t) - \mathcal{T}_\tau v(t)\|_H^2 \le \|v_\tau - v\|^2_{L^2(-T,T,H)} \xrightarrow[\tau\searrow 0]{} 0, \tag{7.12}$$

for all $0 < \tau < T$. While the second addend has already been discussed in (7.10). Hence, we can infer that

$$\int_0^T \|\mathcal{T}_\tau v_\tau(t) - v(t)\|_H^2\,dt \xrightarrow[\tau\searrow 0]{} 0 \tag{7.13}$$

and the proof is complete. □

Finally, we present a fairly standard result concerning the sum of maximal monotone operators. Let us recall some notations previously introduced. We denote by H the space $L^2(\Omega)$, with Ω a bounded domain included in $\mathbb{R}^3$, and by $\mathcal{A}$ the abstract operator prescribed in (2.10). Next, by j we denote a proper, lower semicontinuous and convex function on H, and by $\partial_H j$ the subdifferential of j. Then the following result holds.

Theorem 7.2. *Let $f \in H$. Then, there exists a unique $\chi \in H^2(\Omega) \cap D(j)$ such that*

$$\chi + \mathcal{A}\chi + \partial_H j(\chi) \ni f. \tag{7.14}$$

The above result can be easily proved by approximating the subdifferential operator in (7.14) by its Yosida regularization $(\partial_H j)_\lambda$. We remind that $(\partial_H j)_\lambda$ is maximal monotone and Lipschitz continuous. Hence, we may invoke well known results on the sum of maximal monotone operators (cf. e.g. [8]) and get the existence of a solution $\chi_\lambda \in H^2(\Omega)$ solving the approximated equation. Next, we could perform standard a priori estimates, independent of λ, on the approximated system and get the limit as $\lambda \searrow 0$ by compactness. Finally, uniqueness could be deduced via standard contradiction arguments owing to the monotonicity of the subdifferential operator.

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Elisabetta Chiodaroli, Institut für Mathematik, Universität Zürich, Winterthurerstrasse 190, CH-8057 Zürich, Switzerland

E-mail address: `elisabetta.chiodaroli@math.uzh.ch`